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(54) Title: DRUG THERAPY FOR CELIAC SPRUE

(57) **Abstract:** Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto are decreased by administration of an HLA-binding peptide inhibitor. Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific T cells.

# DRUG THERAPY FOR CELIAC SPRUE

## CROSS-REFERENCE TO RELATED APPLICATIONS

[01] This application claims priority to U.S. Provisional Application 60/380,761 filed May 14, 2002; to U.S. Provisional Application 60/392,782 filed June 28, 2002; and to U.S. Provisional application no. 60/422,933, filed October 31, 2002, and to U.S. Provisional Application 60/428,033, filed November 20, 2002, each of which are herein specifically incorporated by reference.

## BACKGROUND OF THE INVENTION

[02] In 1953, it was first recognized that ingestion of gluten, a common dietary protein present in wheat, barley and rye causes a disease called Celiac Sprue in sensitive individuals. Gluten is a complex mixture of glutamine- and proline-rich gliadin and glutenin molecules and is thought to be responsible for induction of Celiac Sprue. Ingestion of such proteins by sensitive individuals produces flattening of the normally luxurious, rug-like, epithelial lining of the small intestine known to be responsible for efficient and extensive terminal digestion of peptides and other nutrients. Other clinical symptoms of Celiac Sprue include fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, anemia, as well as an enhanced risk for the development of osteoporosis and intestinal malignancies such as lymphoma and carcinoma. The disease has an incidence of approximately 1 in 200 in European populations and is believed to be significantly under diagnosed in other populations.

[03] A related disease is dermatitis herpetiformis, which is a chronic eruption of the skin characterized by clusters of intensely pruritic vesicles, papules, and urticaria-like lesions. IgA deposits occur in almost all normal-appearing and perilesional skin. Asymptomatic gluten-sensitive enteropathy is found in 75 to 90% of patients and in some of their relatives. Onset is usually gradual. Itching and burning are severe, and scratching often obscures the primary lesions with eczematization of nearby skin, leading to an erroneous diagnosis of eczema. Strict adherence to a gluten-free diet for prolonged periods may control the disease in some patients, obviating or reducing the requirement for drug therapy. Dapsone, sulfapyridine, and colchicines are sometimes prescribed for relief of itching.

[04] Celiac Sprue (CS) is generally considered to be an autoimmune disease and the antibodies found in the serum of the patients support the theory that the disease is immunological in nature. Antibodies to tissue transglutaminase (TG2, tTGase or tTG) and gliadin appear in almost 100% of the patients with active CS, and the presence of such antibodies, particularly of the IgA class, has been used in diagnosis of the disease.

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[05]     The large majority of patients express the HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] molecules. It is believed that intestinal damage is caused by interactions between specific gliadin oligopeptides and the HLA-DQ2 or DQ8 antigen, which in turn induce proliferation of T lymphocytes in the sub-epithelial layers. T helper 1 cells and cytokines apparently play a major role in a local inflammatory process leading to villous atrophy of the small intestine.

[06]     At the present time, there is no good therapy for the disease, except to avoid completely all foods containing gluten. Although gluten withdrawal has transformed the prognosis for children and substantially improved it for adults, some people still die of the disease, mainly adults who had severe disease at the outset. A leading cause of death is lymphoreticular disease, especially intestinal lymphoma. It is not known whether a gluten-free diet diminishes this risk. Apparent clinical remission is often associated with histologic relapse that is detected only by review biopsies or by increased titers of antibodies to tTGase (also called EMA antibodies).

[07]     Gluten is so widely used, for example, in commercial soups, sauces, ice creams, hot dogs, and other foodstuffs, that patients need detailed lists of foodstuffs to avoid and expert advice from a dietitian familiar with celiac disease. Ingesting even small amounts of gluten may prevent remission or induce relapse. Supplementary vitamins, minerals, and hematinics may also be required, depending on deficiency. A few patients respond poorly or not at all to gluten withdrawal, either because the diagnosis is incorrect or because the disease is refractory. In the latter case, oral corticosteroids (e.g., prednisone 10 to 20 mg bid) may induce response.

[08]     In view of the serious and widespread nature of Celiac Sprue and the difficulty of removing gluten from the diet, better methods of treatment are of great interest. In particular, there is a need for treatment methods that allow the Celiac Sprue individual to eat gluten-containing foodstuffs without ill effect or at least to tolerate such foodstuffs in small or moderate quantities without inducing relapse. The present invention meets this need for better therapies for Celiac Sprue.

## SUMMARY OF THE INVENTION

[09]     In one aspect, the present invention provides methods for treating Celiac Sprue and/or dermatitis herpetiformis and the symptoms thereof by administration of an HLA-binding peptide inhibitor to the patient. In one embodiment, the HLA-binding peptide inhibitor employed in the method is an analog of an immunogenic gluten peptide, where an immunogenic gluten peptide is altered by the replacement of one or more amino acids, where the replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like. Analogs of

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immunogenic gluten peptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells, are useful agents to treat Celiac Sprue.

[10]     In another aspect, the present invention provides novel HLA-binding peptide inhibitors and methods for treating Celiac Sprue and/or dermatitis herpetiformis by administering those compounds.

[11]     In another aspect, the invention provides pharmaceutical formulations comprising an HLA-binding peptide inhibitor and a pharmaceutically acceptable carrier.   In one embodiment, such formulations comprise an enteric coating that allows delivery of the active agent to the intestine, and the agents are stabilized to resist digestion or acid-catalyzed modification in acidic stomach conditions.   In another embodiment, the formulation also comprises one or more glutenases, as described in U.S. Provisional Application 60/392,782 filed June 28, 2002; and U.S. Provisional Application 60/428,033, filed November 20, 2002, both of which are incorporated herein by reference. The invention also provides methods for the administration of enteric formulations of one or more HLA-binding peptide inhibitors to treat Celiac Sprue.

[12]     In another aspect, the invention provides methods for screening candidate compounds to determine their suitability for use in the subject methods, by assessing the ability of a candidate agent for its ability to bind to HLA molecules, and/or to inhibit the activity of T cells reactive against gluten antigens.

[13]     Methods and compositions are provided for modeling the structure of a soluble (extracellular) domain of human HLA-DQ2 bound to an immunodominant gluten epitope, and for identifying molecules that will compete with the gluten peptide for MHC binding.   In one embodiment, the methods of the invention utilize structural modeling, and the identification and design of molecules having a particular structure.   The structural data provided herein is used for the rational design of drugs that affect immune system activation in Celiac Sprue and/or dermatitis herpetiformis.   Analysis of the crystal structure in conjunction with sequence data identifies residues in the immunogenic gluten peptide that are important for interaction with the MHC molecule, and those that are accessible for interaction with the T cell antigen receptor.   This information provides a basis for rational drug design.

[14]     These and other aspects and embodiments of the invention and methods for making and using the invention are described in more detail in the description of the drawings and the invention, the examples, the claims, and the drawings that follow.

DETAILED DESCRIPTION OF THE EMBODIMENTS

[15]     Celiac Sprue and/or dermatitis herpetiformis are treated by interfering with HLA binding of immunogenic gluten peptides.  Therapeutic benefit can be enhanced in some individuals by increasing the digestion of gluten oligopeptides, whether by pretreatment of foodstuffs to be ingested or by administration of an enzyme capable of digesting the gluten oligopeptides, together with administration of an HLA-binding peptide inhibitor.  Gluten oligopeptides are highly resistant to cleavage by gastric and pancreatic peptidases such as pepsin, trypsin, chymotrypsin, and the like, and their prolonged presence in the digestive tract can induce an autoimmune response. The antigenicity of gluten oligopeptides and the ill effects caused by an immune response thereto can be decreased by administration of an HLA-binding peptide inhibitor.  Such inhibitors are analogs of immunogenic gluten peptides and (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells.

[16]     Methods and compositions are provided for the administration of one or more HLA-binding peptide inhibitors to a patient suffering from Celiac Sprue and/or dermatitis herpetiformis. In some embodiments and for some individuals, the methods of the invention remove the requirement that abstention from ingestion of glutens be maintained to keep the disease in remission.  The compositions of the invention include formulations of tTGase inhibitors that comprise an enteric coating that allows delivery of the agents to the intestine in an active form; the agents are stabilized to resist digestion or alternative chemical transformations in acidic stomach conditions.  In another embodiment, food is pretreated or combined with glutenase, or a glutenase is co-administered (whether in time or in a formulation of the invention) with an HLA-binding peptide inhibitor of the invention.

[17]     The subject methods are useful for both prophylactic and therapeutic purposes. Thus, as used herein, the term "treating" is used to refer to both prevention of disease, and treatment of a pre-existing condition.  The treatment of ongoing disease, to stabilize or improve the clinical symptoms of the patient, is a particularly important benefit provided by the present invention.  Such treatment is desirably performed prior to loss of function in the affected tissues; consequently, the prophylactic therapeutic benefits provided by the invention are also important.  Evidence of therapeutic effect may be any diminution in the severity of disease, particularly diminution of the severity of such symptoms as fatigue, chronic diarrhea, malabsorption of nutrients, weight loss, abdominal distension, and anemia.  Other disease indicia include the presence of antibodies specific for glutens, antibodies specific for tissue transglutaminase, the presence of pro-inflammatory T cells and cytokines, and degradation of the villus structure of the small intestine. Application of the methods and compositions of the invention can result in the improvement of any and all of these disease indicia of Celiac Sprue.

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[18]      Patients that can benefit from the present invention include both adults and children. Children in particular benefit from prophylactic treatment, as prevention of early exposure to toxic gluten peptides can prevent development of the disease into its more severe forms. Children suitable for prophylaxis in accordance with the methods of the invention can be identified by genetic testing for predisposition, e.g. by HLA typing; by family history, and by other methods known in the art. As is known in the art for other medications, and in accordance with the teachings herein, dosages of the HLA-binding peptide inhibitors of the invention can be adjusted for pediatric use.

[19]      Because most proteases and peptidases are unable to hydrolyze the amide bonds of proline residues, the abundance of proline residues in gliadins and related proteins from wheat, rye and barley can constitute a major digestive obstacle for the enzymes involved. This leads to an increased concentration of relatively stable gluten derived oligopeptides in the gut. These stable gluten derived oligopeptides, called "immunogenic oligopeptides" herein, bind to MHC molecules, including HLA HLA-DQ2 or DQ8 molecules, to stimulate an immune response that results in the autoimmune disease aspects of Celiac Sprue. In some cases the enzyme tissue transglutaminase selectively deamidates certain glutamine residues in these peptides, thereby enhancing their potency for the DQ2 ligand binding pocket.

[20]      HLA-binding peptide inhibitors of the present invention are analogs of immunogenic gluten oligopeptides that (i) retain the ability to bind tightly to HLA molecules; (ii) retain the proteolytic stability of these peptides; but (iii) are unable to activate disease-specific or other T cells. The inhibitor may comprise oligomers of analogs. Multivalent gluten derived epitopes have markedly enhanced immunogenicity. Consequently, multivalent oligopeptides analogs can also be expected to have increased potency for MHC molecules. In addition, these longer peptides can be more resistant toward intestinal brush border proteolysis.

[21]      An immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least about 8 residues, and may comprise at least about 10 residues; at least about 11 residues, at least about 12 residues, at least about 13 residues, at least about 14 residues, or more, where the term "residue" refers to naturally occurring amino acids, non-naturally occurring amino acids, and amino acid mimetics or derivatives; and where the gluten peptide is altered by the replacement of one or more amino acids. The replacement may be another naturally occurring amino acid, non-naturally occurring amino acids, modified amino acids, amino acid mimetics, and the like; and may further be derivitized to further reduce the affinity of these ligands for disease-specific T cell receptors. The sequence of immunogenic gluten oligopeptides can be determined by one of skill in the art. Immunogenic gliadin oligopeptides are peptides derived during normal human digestion of gliadins and related storage proteins as described above, from dietary cereals, e.g. wheat, rye, barley, and the

like. Such oligopeptides act as antigens for T cells in Celiac Sprue. For binding to Class II MHC proteins, immunogenic peptides are usually from about 8 to 20 amino acids in length, more usually from about 10 to 18 amino acids. Such peptides may include PXP motifs, such as the motif PQPQLP. Determination of whether an oligopeptide is immunogenic for a particular patient is readily determined by standard T cell activation and other assays known to those of skill in the art.

[22]      Among gluten proteins with potential harmful effect to Celiac Sprue patients are included the storage proteins of wheat, species of which include *Triticum aestivum; Triticum aethiopicum; Triticum baeoticum; Triticum militinae; Triticum monococcum; Triticum sinskajae; Triticum timopheevii; Triticum turgidum; Triticum urartu, Triticum vavilovii; Triticum zhukovskyi; etc.* A review of the genes encoding wheat storage proteins may be found in Colot (1990) <u>Genet Eng</u> (N Y) **12**:225-41. Gliadin is the alcohol-soluble protein fraction of wheat gluten. Gliadins are typically rich in glutamine and proline, particularly in the N-terminal part. For example, the first 100 amino acids of α- and γ-gliadins contain ~35% and ~20% of glutamine and proline residues, respectively. Many wheat gliadins have been characterized, and as there are many strains of wheat and other cereals, it is anticipated that many more sequences will be identified using routine methods of molecular biology. Examples of gliadin sequences include but are not limited to wheat alpha gliadin sequences, for example as provided in Genbank, accession numbers AJ133612; AJ133611; AJ133610; AJ133609; AJ133608; AJ133607; AJ133606; AJ133605; AJ133604; AJ133603; AJ133602; D84341.1; U51307; U51306; U51304; U51303; U50984; and U08287. A sequence of wheat omega gliadin is set forth in Genbank accession number AF280605.

[23]      Among the immunogenic gluten oligopeptides that may be modified to generate an HLA-binding peptide inhibitor are included the peptide sequence QLQPFPQPELPYP; the sequence PQPELPY; the sequence PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ and longer peptides containing such sequences or multiple copies of such sequences. Gliadins, secalins and hordeins contain several PQPQLPY sequences or sequences similar thereto rich in Pro-Gln residues that are high-affinity substrates for tTGase. The tTGase catalyzed deamidation of such sequences increases their affinity for HLA-DQ2, the class II MHC allele present in >90% Celiac Sprue patients. Presentation of these deamidated sequences by DQ2 positive antigen presenting cells effectively stimulates proliferation of gliadin-specific T cells from intestinal biopsies of most Celiac Sprue patients, providing evidence for the proposed mechanism of disease progression in Celiac Sprue.

[24]      Analog oligopeptides of the invention comprise at least one difference in amino acid sequence from a native gluten peptide, by the replacement of an amino acid with a different

amino acid; a non-naturally occurring amino acid, a peptidomimetics, substituted amino acid, and the like. An L-amino acid from the native peptide may be altered to any other one of the 20 L-amino acids commonly found in proteins, any one of the corresponding D-amino acids, rare amino acids, such as 4-hydroxyproline, and hydroxylysine, or a non-protein amino acid, such as β-alanine, ornithine and homoserine. Also included with the scope of the present invention are amino acids that have been altered by chemical means such as methylation (e.g., α-methylvaline), deamidation, amidation of the C-terminal amino acid by an alkylamine such as ethylamine, ethanolamine, and ethylene diamine, and acylation or methylation of an amino acid side chain function (e.g., acylation of the epsilon amino group of lysine), deimination of arginine to citrulline, isoaspartylation, or phosphorylation on serine, threonine, tyrosine or histidine residues. Importantly, each of these altered amino acids provide a functional handle, e.g. amine, alcohol, aryl halide, and the like, which can be regioselectively derivatized to further reduce the affinity of these ligands for disease-specific T cell receptors. Peptide analogs may be further derivatized with substitutions, including, without limitation, ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group, e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. Such derivatives are encompassed by the term "analog".

[25]     The proteolytic stability of gluten oligopeptides can be attributed, at least in part, to the presence of PXP motifs, which are resistant to enzymatic degradation. Preferred analogs of immunogenic gluten oligopeptides will comprise one or more proline residues, and may comprise one or more PXP motifs.

[26]     An immunogenic gluten peptide of particular interest is the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPF, which is described in detail in International Patent Application US03/04743, herein specifically incorporated by reference. This peptide is both immunogenic and highly stable to proteases. T cell epitopes present in the 33-mer peptide include, inter alia, PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY. In one embodiment of the invention, the immunogenic gluten oligopeptide analog is an analog of a peptide that comprises at least one T cell epitope selected from the group consisting of PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PQPELPYPQ; PYPQPELPY and PYPQPQLPY.

[27]     The structure of an immunogenic gluten oligopeptide bound to a presenting molecule, e.g. HLA-DQ2; HLA-DQ8; etc. can be determined, e.g. by crystallography, NMR, etc., and used to identify residues in a peptide that are involved in the binding to the MHC molecule, and that are involved in the binding to a T cell antigen receptor. Residues identified as accessible for interacting with the T cell receptor may be modified to decrease

the interaction, *e.g.* by increasing steric hindrance, altering hydrophilicity or hydrophobicity, *etc.* Residues identified as involved in interaction with the binding cleft of an MHC molecule may be modified to increase the interaction, *e.g.* by incorporating amino acids known to interact strongly with the binding cleft.

[28]     One inhibitor of interest is an oligopeptide or peptidomimetic that comprises the sequence PXPQPELPY, where X is Gly, Ala, Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp, Glu, or any residue that is substantially bulkier or hydrophilic than Phe. Examples of suitable modifications include ethers, amines, esters, amides, carbonates, carbamates, carbazates, ureas and C-C coupled derivatives. Other examples include oxidation of alcohols to ketones, followed by further modifications of the resulting carbonyl group (e.g. via preparation of oximes) or the carbon atom adjacent to the ketone. The peptide may comprise modifications that increase binding potency to an MHC molecule, by varying residues that facilitate peptide docking into the binding cleft. Examples of such residues include Gln-4, Glu-6, Leu-7, and Tyr-9 (numbering based on the epitope PFPQPELPY). Each of these residues interacts closely with several residues in the DQ2 binding pocket. By using structure-based molecular design methods, these interactions can be optimized.

[29]     Another inhibitor of interest is a oligopeptide or peptidomimetic that comprises the sequence PFPQX$_1$ELX$_2$Y, where X$_1$ and X$_2$ are independently selected from 4-hydroxy-Pro (either isomer at C-4), 4-amino-Pro (either isomer atC-4), or 3-hydroxy-Pro (either isomer atC-3), and proline, with the proviso that at least one of X$_1$ and X$_2$ is a residue other than proline.

[30]     Peptides and peptide analogs may be synthesized by standard chemistry techniques, including synthesis by automated procedure. In general, peptide analogs are prepared by solid-phase peptide synthesis methodology which involves coupling each protected amino acid residue to a resin support, preferably a 4-methylbenzhydrylamine resin, by activation with dicyclohexylcarbodiimide to yield a peptide with a C-terminal amide. Alternatively, a chloromethyl resin (Merrifield resin) may be used to yield a peptide with a free carboxylic acid at the C-terminus. After the last residue has been attached, the protected peptide-resin is treated with hydrogen fluoride to cleave the peptide from the resin, as well as deprotect the side chain functional groups. Crude product can be further purified by gel filtration, HPLC, partition chromatography, or ion-exchange chromatography.

[31]     The present invention provides crystals and structures of HLA-DQ2 bound to antigen, where the antigen is an immunogenic gluten peptide QLQPFPQPELPYP, which may be referred to for brevity as an "HLA-DQ2/peptide complex". The structures and structural coordinates are useful in structural homology deduction, and in developing and

screening agents that affect the gluten antigen presentation and immunogenicity. The structure information may be provided in a computer readable form, *e.g.* as a database of atomic coordinates, or as a three-dimensional model. The structures are useful, for example, in modeling interactions of the HLA molecule with the antigen, effect of inhibitors, *etc.* The structures are also used to identify molecules that bind to or otherwise interact with structural elements. One aspect of the present invention provides crystals of the HLA-DQ2/peptide complex, which can effectively diffract X-rays for the determination of the atomic coordinates.

[32]     The present invention further includes methods of using the structural information provided herein to derive a detailed structure of related peptide binding interactions, particularly other gluten peptides, or analogs and mimetics thereof. Such structural homology determination may utilize modeling, alone or in combination with structure determination.

[33]     The present invention provides three-dimensional coordinates for the HLA-DQ2/peptide complex. Such a data set may be provided in computer readable form. Methods of using such coordinates (including in computer readable form) in drug assays and drug screens as exemplified herein, are also part of the present invention. In a particular embodiment of this type, the coordinates contained in the data set can be used to identify potential modulators of the HLA-DQ2/peptide complex, including molecules that mimic the binding of the peptide to the HLA molecule, but which lack, or are substantially diminished in the ability to stimulate a T cell response.

[34]     In one embodiment, a potential agent for modulation of HLA-DQ2/peptide complex is selected by performing rational drug design with the three-dimensional coordinates determined for the crystal structures. Preferably the selection is performed in conjunction with computer modeling. Rational design may also be used in the genetic modification of immunogenic peptides by modeling the potential effect of a change in the amino acid sequence.

[35]     Computer analysis may be performed with one or more of the computer programs including: GRASP, O (Jones *et al.* (1991) Acta Cryst. **A47**:110); QUANTA, CHARMM, INSIGHT, SYBYL, MACROMODEL; ICM, and CNS (Brunger *et al.* (1998) Acta Cryst. **D54**:905). In a further embodiment of this aspect of the invention, an initial drug screening assay is performed using the three-dimensional structure so obtained, preferably along with a docking computer program. Such computer modeling can be performed with one or more Docking programs such as DOC, GRAM and AUTO DOCK. See, for example, Dunbrack *et al.* (1997) Folding & Design **2**:27-42.

[36]     It should be understood that in the drug screening and protein modification assays provided herein, a number of iterative cycles of any or all of the steps may be performed to

optimize the selection. For example, assays and drug screens that monitor the activity of the T cells in the presence and/or absence of a potential inhibitor are also included in the present invention and can be employed as an assay or drug screen, usually as a single step in a multi-step protocol.

[37]     The structure of the HLA-DQ2/peptide complex is useful in the design of agents that mimic the activity and/or specificity of the binding interaction. The structures encoded by the data may be computationally evaluated for an ability to associate with chemical entities. This provides insight into an element's ability to associate with chemical entities. Chemical entities that are capable of associating with these domains may alter immunogenicity. Such chemical entities are potential drug candidates. Alternatively, the structure encoded by the data may be displayed in a graphical format. This allows visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities.

[38]     In one embodiment of the invention, an invention is provided for evaluating the ability of a chemical entity to associate with any of the molecules or molecular complexes set forth above. This method comprises the steps of employing computational means to perform a fitting operation between the chemical entity and the interacting surface of the polypeptide or nucleic acid; and analyzing the results of the fitting operation to quantify the association. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes. Molecular design techniques are used to design and select chemical entities, including inhibitory compounds, capable of binding to the HLA molecule, or to the gluten peptide. Such chemical entities may interact directly with certain key features of the structure.

[39]     It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a competitive binding agent. In fact, it is only those few atoms that shape the loops and actually form important contacts that are likely to be important for activity. Those skilled in the art will be able to identify these important atoms based on the structure model of the invention, which can be constructed using the structural data herein.

[40]     The design of compounds that bind to HLA-DQ2 according to this invention generally involves consideration of two factors. First, the compound must be capable of either competing for binding with an immunogenic gluten peptide; or physically and structurally associating with the HLA-DQ2 domains. Non-covalent molecular interactions important in this association include hydrogen bonding, van der Waals interactions, hydrophobic interactions and electrostatic interactions.

[41]     The compound must be able to assume a conformation that allows it to interact with the binding pocket. Although certain portions of the compound will not directly participate in

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these associations, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity in relation to all or a portion of the binding pocket, or the spacing between functional groups of an entity comprising several interacting chemical moieties.

[42]      Computer-based methods of analysis fall into two broad classes: database methods and *de novo* design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional data. In *de novo* design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, *e.g.* data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atom-by-atom manner or by assembling stored small molecular fragments. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within the interacting surface of the RNA. Docking may be accomplished using software such as Quanta (Molecular Simulations, San Diego, CA) and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

[43]      Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include: SmoG, GRID (Goodford (1985) J. Med. Chem., 28, pp. 849-857; Oxford University, Oxford, UK; MCSS (Miranker *et al.* (1991) Proteins: Structure, Function and Genetics, 11, pp. 29-34; Molecular Simulations, San Diego, CA); AUTODOCK (Goodsell *et al.*, (1990) Proteins: Structure, Function, and Genetics, 8, pp. 195-202; Scripps Research Institute, La Jolla, Calif.); and DOCK (Kuntz *et al.* (1982) J. Mol. Biol., 161:269-288; University of California, San Francisco, Calif.)

[44]      Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates. Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett *et al.* (1989) In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196; University of California, Berkeley, Calif.); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif); and HOOK (available from Molecular Simulations, San Diego, CA).

[45]     Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

[46]     Once the binding entity has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties.  Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group.  It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit by the same computer methods described above.

[47]     Another approach made possible and enabled by this invention, is the computational screening of small molecule databases. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy.  Generally the tighter the fit, the lower the steric hindrances, and the greater the attractive forces, the more potent the potential modulator since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interact as well with other proteins. This will minimize potential side effects due to unwanted interactions with other proteins.

[48]     Compounds of interest can be systematically modified by computer modeling programs until one or more promising potential analogs are identified.  In addition systematic modification of selected analogs can then be systematically modified by computer modeling programs until one or more potential analogs are identified. Alternatively a potential modulator could be obtained by initially screening a random peptide library, for example one produced by recombinant bacteriophage.  A peptide selected in this manner would then be systematically modified by computer modeling programs as described above, and then treated analogously to a structural analog.

[49]     Once a potential modulator/inhibitor is identified it can be either selected from a library of chemicals as are commercially available from most large chemical companies including Merck, GlaxoWelcome, Bristol Meyers Squib, Monsanto/Searle, Eli Lilly, Novartis and Pharmacia UpJohn, or alternatively the potential modulator may be synthesized *de novo*. The *de novo* synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design.

[50]     The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally

relevant portion of the compound of interest. For drugs, the functionally relevant portion may be referred to as a pharmacophore, *i.e.* an arrangement of structural features and functional groups important for biological activity. Not all identified compounds having the desired pharmacophore will act as a modulator of inflammation. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds that must be tested to identify an actual inhibitor.

[51]    In order to determine the biological activity of a candidate pharmacophore it is preferable to measure biological activity at several concentrations of candidate compound. The activity at a given concentration of candidate compound can be tested in a number of ways.

[52]    For example, an HLA molecule can be attached to a solid support. Methods for placing proteins on a solid support are well known in the art and include such steps as linking biotin to the protein, and linking avidin to the solid support. The solid support can be washed to remove unreacted species. A solution of a labeled candidate agent can be contacted with the solid support. The solid support is washed again to remove the potential modulator not bound to the support. The amount of labeled potential modulator remaining with the solid support and thereby bound to the protein can be determined. Alternatively, or in addition, the dissociation constant between the labeled candidate agent and the protein can be determined.

[53]    Crystals of the binding complex of the present invention can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. The crystals may be shrunk by transfer into solutions of different composition, *e.g.* by the addition of metal ions such as $Mn^{2+}$, $Pb^{2+}$, *etc*. Crystals may also be generated that include cofactors, substrates, candidate inhibitors, and the like, that interact with the protein, *e.g.* by cocrystallization of soaking protein crystals in a solution comprising an inhibitor or other agent.

[54]    Alternative methods may also be used. For example, crystals can be characterized by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source. Methods of characterization include, but are not limited to, precision photography, oscillation photography and diffractometer data collection. Selenium-methionine may be used as described in the examples provided herein, or alternatively a heavy metal derivative data set (e.g., using PCMB) may be used in place of the selenium-methionine derivatization.

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[55]      Electron density maps may be built from crystals using phase information from multiple isomorphous heavy-atom derivatives, molecular replacement or selenomethionine incorporated multiwavelength anomalous disperson technique.  Model building is facilitated by the use of sequence markers, especially selenomethionine residues.  Anomalous difference Fourier maps may be calculated with data from selenomethionine-substituted HLA-DQ2/ GLUTEN EPITOPE and with experimental multiple isomorphous replacement with anomalous scattering (MIRAS) phases (Hemming and Edwards (2000) J. Biol. Chem. 275:2288).  Maps are improved by phase combination, where MIRAS phases are combined by the program SIGMAA (Jones *et al.*, *supra*.)  Phase combination may be followed by solvent flattening with DM (Carson (1997) Methods Enzymol. 277:493).  Improved maps may be obtained by combination of the MIRAS phases with improved phases from combined polyalanine and atomic models in an iterative process.  The model can be refined by classical positional and B-factor minimization, and with manual rebuilding.

[56]      HLA-DQ2/peptide complex structure models and databases of structure information are provided.  The structural models find use in determining the structure of related and/or analogous peptide complexes.  In some cases, modeling will be based on the provided structure.  In other embodiments, modeling will utilize the provided structure in combination with features present in homologous and/or related structures, where relationship may be defined by protein sequence similarity, or structural similarity, e.g. in the presence of specific features as described above.

[57]      The structure model may be implemented in hardware or software, or a combination of both.  For most purposes, in order to use the structure coordinates generated for the structure, it is necessary to convert them into a three-dimensional shape.  This is achieved through the use of free or commercially available software that is capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structure coordinates.

[58]      In one embodiment of the invention, a machine-readable storage medium is provided, the medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of any of the structures of this invention that have been described above.  Specifically, the computer-readable storage medium is capable of displaying a graphical three-dimensional representation of the HLA-DQ2/peptide complex.

[59]      Thus, in accordance with the present invention, data providing structural coordinates, alone or in combination with software capable of displaying the resulting three dimensional structure of the complex, portions thereof, and their structurally similar analogs, is stored in a machine-readable storage medium.  Such data may be used for a variety of

purposes, such as drug discovery, analysis of interactions between cellular components during translation, modeling of vaccines, and the like.

[60] Preferably, the invention is implemented in computer programs executing on programmable computers, comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

[61] Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

[62] Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

[63] The HLA-binding peptide inhibitors are incorporated into a variety of formulations for therapeutic administration. In one aspect, the agents are formulated into pharmaceutical compositions by combination with appropriate, pharmaceutically acceptable carriers or diluents, and may be formulated into preparations in solid, semi-solid, liquid or gaseous forms, such as tablets, capsules, powders, granules, ointments, solutions, suppositories, injections, inhalants, gels, microspheres, and aerosols. As such, administration can be achieved in various ways, usually by oral administration. The HLA-binding peptide inhibitors may be systemic after administration or may be localized by virtue of the formulation, or by the use of an implant that acts to retain the active dose at the site of implantation.

[64] In pharmaceutical dosage forms, the HLA-binding peptide inhibitors may be administered in the form of their pharmaceutically acceptable salts, or they may also be used alone or in appropriate association, as well as in combination with other pharmaceutically active compounds. The agents may be combined, as previously described, to provide a cocktail of activities. The following methods and excipients are merely exemplary and are in no way limiting.

[65]     For oral preparations, the agents can be used alone or in combination with appropriate additives to make tablets, powders, granules or capsules, for example, with conventional additives, such as lactose, mannitol, corn starch or potato starch; with binders, such as crystalline cellulose, cellulose derivatives, acacia, corn starch or gelatins; with disintegrators, such as corn starch, potato starch or sodium carboxymethylcellulose; with lubricants, such as talc or magnesium stearate; and if desired, with diluents, buffering agents, moistening agents, preservatives and flavoring agents.

[66]     In one embodiment of the invention, the oral formulations comprise enteric coatings, so that the active agent is delivered to the intestinal tract. Enteric formulations are often used to protect an active ingredient from the strongly acid contents of the stomach. Such formulations are created by coating a solid dosage form with a film of a polymer that is insoluble in acid environments, and soluble in basic environments. Exemplary films are cellulose acetate phthalate, polyvinyl acetate phthalate, hydroxypropyl methylcellulose phthalate and hydroxypropyl methylcellulose acetate succinate, methacrylate copolymers, and cellulose acetate phthalate.

[67]     Other enteric formulation comprise engineered polymer microspheres made of biologically erodable polymers, which display strong adhesive interactions with gastrointestinal mucus and cellular linings, can traverse both the mucosal absorptive epithelium and the follicle-associated epithelium covering the lymphoid tissue of Peyer's patches. The polymers maintain contact with intestinal epithelium for extended periods of time and actually penetrate it, through and between cells. See, for example, Mathiowitz *et al.* (1997) Nature 386 (6623): 410-414. Drug delivery systems can also utilize a core of superporous hydrogels (SPH) and SPH composite (SPHC), as described by Dorkoosh *et al.* (2001) J Control Release 71(3):307-18.

[68]     Formulations are typically provided in a unit dosage form, where the term "unit dosage form," refers to physically discrete units suitable as unitary dosages for human subjects, each unit containing a predetermined quantity of glutenase calculated in an amount sufficient to produce the desired effect in association with a pharmaceutically acceptable diluent, carrier or vehicle. The specifications for the unit dosage forms of the present invention depend on the particular complex employed and the effect to be achieved, and the pharmacodynamics associated with each complex in the host.

[69]     The pharmaceutically acceptable excipients, such as vehicles, adjuvants, carriers or diluents, are readily available to the public. Moreover, pharmaceutically acceptable auxiliary substances, such as pH adjusting and buffering agents, tonicity adjusting agents, stabilizers, wetting agents and the like, are readily available to the public.

## METHODS OF TREATMENT

[70]     The subject methods are used to treat individuals suffering from Celiac Sprue and/or dermatitis herpetiformis, by administering an effective dose through a pharmaceutical formulation.  Diagnosis of suitable patients may utilize a variety of criteria known to those of skill in the art.   A quantitative increase in antibodies specific for gliadin, and/or tissue transglutaminase is indicative of the disease.  Family histories and the presence of the HLA alleles HLA-DQ2 [DQ(a1*05, b1*02)] and/or DQ8 [DQ(a1*03, b1*0302)] are indicative of a susceptibility to the disease.  Specific peptide analogs may be administered therapeutically to decrease inflammation, and/or to induce antigen-specific tolerance to treat autoimmunity.  Methods for the delivery of peptides that are altered from a native peptide are known in the art.   Alteration of native peptides with selective changes of crucial residues can induce unresponsiveness or change the responsiveness of antigen-specific autoreactive T cells.

[71]     The therapeutic effect may be measured in terms of clinical outcome, or may rely on immunological or biochemical tests.  Suppression of the deleterious T-cell activity can be measured by enumeration of reactive Th1 cells, by quantitating the release of cytokines at the sites of lesions, or using other assays for the presence of autoimmune T cells known in the art. Alternatively, one may look for a reduction in symptoms of a disease.

[72]     Various methods for administration may be employed.   The dosage of the therapeutic formulation will vary widely, depending upon the nature of the disease, the frequency of administration, the manner of administration, the clearance of the agent from the host, and the like.  Such treatment could either be before meals or on a once-a-day basis or on a once-a-week basis, depending on the half-life of the inhibitor.  A typical dose is at least about 1 µg, usually at least about 10 µg, more usually at least about 0.1 mg, and not more than about 10 mg, usually not more than about 1 mg. Enteric coating of these peptides may also enhance their lifetimes in the gut, thereby permitting delivery to the proximal and distal small intestinal tissue.  Treatment of other autoimmune disorders such as Type I diabetes with such ligands may involve oral, intravenous or intramuscular administration.  The initial dose may be larger, followed by smaller maintenance doses. The dose may be administered as infrequently as weekly or biweekly, or more often fractionated into smaller doses and administered daily, with meals, semi-weekly, *etc.* to maintain an effective dosage level.

[73]     The HLA-binding peptide inhibitors of the invention may be administered in the treatment of Type 1 diabetes (IDDM).  IDDM and celiac disease are both immunologic disorders where specific HLA alleles are associated with disease risk.  Transglutaminase autoantibodies can be found in some patients with IDDM. The prevalence of transglutaminase autoantibodies is higher in diabetic patients with HLA DQ2 or DQ8.

[74]     Human type I or insulin-dependent diabetes mellitus (IDDM) is characterized by autoimmune destruction of the β cells in the pancreatic islets of Langerhans. The depletion of β cells results in an inability to regulate levels of glucose in the blood. Overt diabetes occurs when the level of glucose in the blood rises above a specific level, usually about 250 mg/dl. In humans a long presymptomatic period precedes the onset of diabetes. During this period there is a gradual loss of pancreatic beta cell function. IDDM is currently treated by monitoring blood glucose levels to guide injection, or pump-based delivery, of recombinant insulin. Diet and exercise regimens contribute to achieving adequate blood glucose control. The inhibitors of the invention may be administered alone, or in combination with other therapies. The route of administration may be oral, as described for treatment of Celiac Sprue, or may be injected, *e.g.* i.v., i.m., *etc.* Administration may be performed during the pre-symptomatic phase, or in overt diabetes.

EXPERIMENTAL

Example

[75]     It has long been known that the principal toxic components of wheat gluten are a family of closely related Pro-Gln rich proteins called gliadins. Recent reports have suggested that peptides from a short segment of α-gliadin appear to account for most of the gluten-specific recognition by CD4+ T cells from Celiac Sprue patients. These peptides are substrates of tissue transglutaminase (tTGase), the primary auto-antigen in Celiac Sprue, and the products of this enzymatic reaction bind to the class II HLA DQ2 molecule. This "immunodominant" region of α-gliadin is part of an unusually long proteolytic product generated by the digestive process that: (a) is exceptionally resistant to further breakdown by gastric, pancreatic and intestinal brush border proteases; (b) is the highest specificity substrate of human tissue transglutaminase (tTGase) discovered to date; (c) contains at least six overlapping copies of epitopes known to be recognized by patient derived T cells; (d) stimulates representative T cell clones that recognize these epitopes with sub-micromolar efficacy; and (e) has homologs in proteins from all toxic foodgrains but no homologs in non-toxic foodgrain proteins.

[76]     *Identification of stable peptides from gastric protease, pancreatic protease and brush border membrane peptidase catalyzed digestion of recombinant α2-gliadin:* α2-gliadin, a representative α-gliadin (Arentz-Hansen et al. (2000) Gut **46**:46), was expressed in recombinant form and purified from E. coli. The α2-gliadin gene was cloned in pET28a plasmid (Novagen) and transformed into the expression host BL21(DE3) (Novagen). The transformed cells were grown in 1-liter cultures of LB media containing 50 μg/ml of

kanamycin at 37 °C until the OD600 0.6-1 was achieved. The expression of α2-gliadin protein was induced with the addition of 0.4 mM isopropyl α-D-thiogalactoside (Sigma) and the cultures were further incubated at 37 °C for 20 hours. The cells expressing the recombinant α2-gliadin were centrifuged at 3600 rpm for 30 minutes. The pellet was resuspended in 15 ml of disruption buffer (200 mM sodium phosphate; 200 mM NaCl; 2.5 mM DTT; 1.5 mM benzamidine; 2.5 mM EDTA; 2 mg/L pepstatin; 2 mg/L leupeptin; 30% v/v glycerol) and lysed by sonication (1 minute; output control set to 6). After centrifugation at 45000g for 45 min, the supernatant was discarded and the pellet containing gliadin protein was resuspended in 50 ml of 7M urea in 50 mM Tris (pH = 8.0). The suspension was again centrifuged at 45000g for 45 min and the supernatant was harvested for purification. The supernatant containing α2-gliadin was incubated with 1 ml of nickel-nitrilotriacetic acid resin (Ni-NTA; Qiagen) overnight and then batch-loaded on a column with 2 ml of Ni-NTA. The column was washed with 7M urea in 50 mM Tris (pH = 8.0) and α2-gliadin was eluted with 200 mM imidazole, 7 M urea in 50 mM Tris (pH = 4.5). The fractions containing α2-gliadin were pooled into a final concentration of 70% ethanol solution and two volumes of 1.5M NaCl were added to precipitate the protein. The solution was incubated at 4 °C overnight and the final precipitate was collected by centrifugation at 45000 g for 30 min, rinsed in water, and re-centrifuged to remove the urea. The final purification step of the α-2 gliadin was developed with reverse-phase HPLC. The Ni-NTA purified protein fractions were pooled in 7 M urea buffer and injected to a Vydac (Hesperia, CA) polystyrene reverse-phase column (i.d. 4.6 mm × 25 cm) with the starting solvent (30% of solvent B: 1:1 HPLC-grade acetonitrile/isopropanol : 0.1% TFA). Solvent A was an aqueous solution with 0.1% TFA. The separation gradient extended from 30–100% of solvent B over 120 min at a flow rate of 0.8 ml/min.

Table 2, Amount of Peptides Digested after 15 hours

|  | 33-mer | Control A | Control B |
|---|---|---|---|
| H1P0 | <20% | >90% | >90% |
| H2P0 | <20% | >61% | >85% |
| H3P0 | <20% | >87% | >95% |
| H4P0 | <20% | >96% | >95% |
| H5P0 | <20% | >96% | >95% |

[77]     The purity of the recombinant gliadin was >95%, which allowed for facile identification and assignment of proteolytic products by LC-MS/MS/UV. Although many previous studies utilized pepsin/trypsin treated gliadins, it was found that, among gastric and pancreatic proteases, chymotrypsin played a major role in the breakdown of α2-gliadin,

resulting in many small peptides from the C-terminal half of the protein and a few longer (>8 residues) peptides from the N-terminal half, the most noteworthy being a relatively large fragment, the 33-mer LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPF (residues 57-89). This peptide was of particular interest for two reasons: (a) Whereas most other relatively stable proteolytic fragments were cleaved to smaller fragments when the reaction times were extended, the 33-mer peptide remained intact despite prolonged exposure to proteases; and (b) three distinct patient-specific T cell epitopes identified previously are present in this peptide, namely, PFPQPQLPY, PQPQLPYPQ (3 copies), and PYPQPQLPY (2 copies).

[78]     To establish the physiological relevance of this peptide, composite gastric/pancreatic enzymatic digestion of α2 gliadin was then examined.  As expected, enzymatic digestion with pepsin (1:100 w/w ratio), trypsin (1:100), chymotrypsin (1:100), elastase (1:500) and carboxypeptidase (1:100) was quite efficient, leaving behind only a few peptides longer than 9 residues (the minimum size for a peptide to show class II MHC mediated antigenicity).  In addition to the above-mentioned 33-mer, the peptide WQIPEQSR was also identified, and was used as a control in many of the following studies.

[79]     The small intestinal brush-border membrane (BBM) enzymes are known to be vital for breaking down any remaining peptides from gastric/pancreatic digestion into amino acids, dipeptides or tripeptides for nutritional uptake.  Therefore a comprehensive analysis of gliadin metabolism also required investigations into BBM processing of gliadin peptides of reasonable length derived from gastric and pancreatic protease treatment.  BBM fractions were prepared from rat small intestinal mucosa. The specific activities of known BBM peptidases were verified to be within the previously reported range.  Whereas the half-life of disappearance of WQIPEQSR was ~60 min in the presence of 12 ng/μl BBM protein, the half-life of LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPF digestion was >20 h. Therefore, the latter peptide remains intact throughout the digestive process in the stomach and upper small intestine, and is poised to act as a potential antigen for T cell proliferation and intestinal toxicity in genetically susceptible individuals.


## Example 2

The 33-mer gliadin peptide is an excellent substrate for tTGase, and the resulting product is a highly potent activator of patient-derived T cells: A number of recent studies have demonstrated that regiospecific deamidation of immunogenic gliadin peptides by tTGase increases their affinity for HLA-DQ2 as well as the potency with which they activate patient-derived gluten-specific T cells.  It has been shown the specificity of tTGase for certain short antigenic peptides derived from gliadin is higher than its specificity toward its physiological target site in fibronectin, for example, the specificity of tTGase for the α-gliadin

derived peptide PQPQLPYPQPQLPY is 5-fold higher than that for its target peptide sequence in fibrinogen, its natural substrate. The kinetics and regiospecificity of deamidation of the 33-mer α-gliadin peptide identified as above were therefore measured. The $k_{cat}/K_M$ was higher than that reported for any peptide studied thus far: kcat / KM = 440 min-1mM-1 for LQLQPFPQPQLPYPQPQLPYPQPQLPYPQPQPF compared to kcat / KM = 82 min-1mM-1 for PQPQLPY and kcat / KM = 350 min-1mM-1 for PQPQLPYPQPQLPY.

[80]     Moreover,       LC-MS-MS        analysis        revealed         that LQLQPFPQP**Q**LPYPQPQLPYPQP**Q**LPYPQPQPF was selectively deamidated by tTGase at the underlined residues. Since tTGase activity is associated with the brush border membrane of intestinal enterocytes, it is likely that dietary uptake of even small quantities of wheat gluten will lead to the build-up of sufficient quantities of this 33-mer gliadin peptide in the intestinal lumen so as to be recognized and processed by tTGase.

[81]     *Structural characteristics of the 33-mer gliadin peptide and its naturally occurring homologs:* Sequence alignment searches using BLASTP in all non-redundant protein databases revealed several homologs (E-value < 0.001) of the 33-mer gliadin peptide. Interestingly, foodgrain derived homologs were only found in gliadins (from wheat), hordeins (from barley) and secalins (from rye), all of which have been proven to be toxic to Celiac patients (Figure 7). Nontoxic foodgrain proteins, such as avenins (in oats), rice and maize, do not contain homologous sequences to the 33-mer gliadin. In contrast, a BLASTP search with the entire α2-gliadin sequence identified foodgrain protein homologs from both toxic and nontoxic proteins. Based on available information regarding the substrate specificities of gastric, pancreatic and BBM proteases and peptidases, it is predicted that, although most gluten homologs to the 33-mer gliadin peptide contained multiple proteolytic sites and are therefore unlikely to be completely stable toward digestion, several sequences from wheat, rye and barley are expected to be comparably resistant to gastric and intestinal proteolysis. The stable peptide homologs to the 33-mer α2-gliadin peptide are QPQPFPPQLPYPQTQPFPPQQPYPQPQPQYPQPQ (from α1- and α6-gliadins); QQQPFPQQPIPQQPQPYPQQPQPYPQQPFPPQQPF (from B1 hordein); QPFPQPQQTFPQQPQLPFPQQPQQPFPQPQ (from γ-gliadin); VQWPQQQPVPQPHQPF (from γ-gliadin), VQGQGIIQPQQPAQ (from γ-gliadin), FLQPQQPFPQQPQQPYPQQPQQPFPQ (from γ-gliadin), FSQPQQQFPQPQQPQQSFPQQQPP (from γ-gliadin), QPFPQPQQPTPIQPQQPFPQRPQQPFPQPQ (from ω-secalin). These stable peptides are all located at the N-terminal region of the corresponding proteins. The presence of proline residues after otherwise cleavable residues in these peptides would contribute to their proteolytic stability.

[82]      The unique primary sequence of the 33-mer gliadin peptide also had homologs among a few non-gluten proteins.  Among the strongest homologs were internal sequences from pertactin (a highly immunogenic protein from *Bordetella pertussis*) and a mammalian inositol-polyphosphate 5-phosphatase of unknown function.   In both cases available information suggested that the homology could have biologically relevance.  For example, the region of pertactin that is homologous to the 33-mer gliadin peptide is known to be part of the immunodominant segment of the protein.   In the case of the homologous phosphatase, the corresponding peptide region of the phosphatase is known to be responsible for vesicular trafficking of the phosphatase to the cytoplasmic Golgi.  In analogy with the current picture of how gliadin peptides are presented to HLA-DQ2 via a tTGase mediated pathway, these Pro-Gln-rich segments of both pertactin and the phosphatase are likely to be good tTGase substrates.

## Example 3

[83]      *X-ray Crystallographic Analysis of soluble HLA-DQ2.*   The soluble extracellular domains of the α- and β-chains of HLA-DQ2 were co-expressed in insect cells using a baculovirus expression system (pAcAB3 vector, BD Biosciences). The DNA sequence of the engineered α- and β-chains is provided in SEQ ID NO:1 and SEQ ID NO:2.  The β-chain is fused to a sequence encoding the epitope QLQPFPQPELPY at its N-terminal end, and to a biotin recognition sequence at its C-terminal end.   Both subunits are also fused to complementary leucine zipper sequences at their C-terminal ends.   Since a Factor Xa proteolysis site is engineered between the leucine zipper sequences and the DQ2 subunits, prior to crystallization the leucine zippers were removed from DQ2 by Factor Xa digestion.

[84]      Initial purification of the DQ2 heterodimer from the culture medium was performed on an immunoaffinity column containing an anti-DQ2 monoclonal antibody (2.12.E11) bound to a Protein A Sepharose CL-4B column.   Subsequently DQ2 was treated with Factor Xa, and purified from the digestion mixture by anion-exchange chromatography followed by size-exclusion chromatography, and concentrated to 4 mg/ml in 25 mM Tris-HCl, pH 8.0. Crystals of the DQ2-epitope complex were obtained using the hanging drop method. Typically, 2 μL of protein solution (2~4 mg/ml DQ2, 25 mM Tris-HCl, pH 8.0) and 2 μL of precipitant buffer (200 mM ammonium acetate, 40 mM ammonium sulfate, 4% ethylene glycol, 22~26% PEG 3350) were combined in a single drop hanging over 1 mL of precipitant buffer at room temperature.  Small crystals appeared within three days and grew to full size in two weeks.

[85]      For data collection, crystals were transferred to a cryoprotectant solution (mother liquor containing 28% ethylene glycol) for 2 hours, and then flash cooled at 100K in liquid nitrogen.  X-ray diffraction data were collected from a single crystal to 2.22 Å resolution at

beamline 11-1 of the Stanford Synchrotron Radiation Laboratory using a Quantum 315 CCD detector. Oscillation images were processed with DENZO and data reduction was carried out with SCALEPACK.

[86]     The structure of DQ2-epitope complex was determined by molecular replacement using the program AMoRe in the CCP4 suite of programs. The 2.4 Å resolution structure of insulin peptide-HLA-DQ8 complex (RCSB accession code: 1JK8) minus the insulin peptide and solvent molecules was used as the search model. After initial refinement with the maximum likelihood function of program REFMAC, iterative cycles of refinement including simulated annealing, temperature factor refinement, and energy minimization were made with the program CNS. Model building and correction were performed using $\sigma_A$-weighted $F_o$-$F_c$ and $2F_o$-$F_c$ electron density maps with the program O. The current model has $R$-factor of 0.2209 with a $R_{free}$ of 0.2793 at 2.22 Å resolution. Analysis of the Ramachandran plot generated using the program PROCHECK shows that 91.2 % of residues are in most favored regions, 7.9 % are in additional allowed regions, 0.5 % are in generously allowed regions, and 0.5 % are in disallowed regions.

[87]     There are two molecules of DQ2-epitope in the asymmetric unit. In the first complex, α-chain of DQ2, β-chain of DQ2, and the alpha-I epitope peptide (sequence QLQPFPQPELPY) are designated A, B, and C respectively. In the second complex, α-chain, β-chain, and epitope peptide are designated D, E, and F respectively. The model includes 354 water molecules (name: HOH) and 4 ethylene glycol molecules (name: EDO).

[88]     Thr-106—His-112 region in chain B and Arg-105—His-112 region in chain E are disordered and thus absent from the model. Superposition of the DQ8 structure suggests that these regions form an extended loop. Side chain conformation of the following residues are undefined due to weak electron density in the corresponding region and therefore only their backbone atoms are included in the model: Asp-135 (in chain B), Leu-2, Gln-3, Tyr-12 (in chain C), Asp-135, Gln-136 (in chain E), and Leu-2, Gln-3 (in chain F).

[89]     *Structure-based design of DQ2 binding peptide inhibitors.* The crystal structure of the DQ2-epitope complex reveals precisely which atoms in the peptide QLQPFPQPELPYP point outward (by inference into the T cell receptor binding pocket). Substitutions at these atoms can yield altered peptide ligands that retain the ability to bind tightly to DQ2 but are no longer able to allow docking of the DQ2-peptide complex into disease specific T cell receptors.

[90]     The coordinate of the structure are as follows:

### Coordinates

```
REMARK peptide link removed (applied DPEP): from B    105  to B    113
REMARK peptide link removed (applied DPEP): from E    104  to E    113
REMARK disulphide added: from A    107  to A    163
REMARK disulphide added: from B     15  to B     79
REMARK disulphide added: from B    117  to B    173
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REMARK disulphide added: from D    107   to D      163
REMARK disulphide added: from E     15   to E       79
REMARK disulphide added: from E    117   to E      173
REMARK DATE:25-Apr-03  13:00:06       created by user: kim
REMARK VERSION:1.0
ATOM        1   CB  VAL A   2     31.060   3.851   4.095  1.00 39.43       A
ATOM        2   CG1 VAL A   2     30.078   2.835   3.531  1.00 40.06       A
ATOM        3   CG2 VAL A   2     30.370   5.185   4.344  1.00 39.97       A
ATOM        4   C   VAL A   2     30.653   3.406   6.542  1.00 36.80       A
ATOM        5   O   VAL A   2     29.644   2.702   6.527  1.00 38.25       A
ATOM        6   N   VAL A   2     32.189   1.926   5.235  1.00 36.80       A
ATOM        7   CA  VAL A   2     31.684   3.321   5.414  1.00 37.95       A
ATOM        8   N   ALA A   3     30.910   4.267   7.523  1.00 34.99       A
ATOM        9   CA  ALA A   3     30.003   4.416   8.658  1.00 32.94       A
ATOM       10   CB  ALA A   3     30.325   3.368   9.721  1.00 33.34       A
ATOM       11   C   ALA A   3     30.094   5.805   9.263  1.00 30.81       A
ATOM       12   O   ALA A   3     30.980   6.583   8.914  1.00 29.57       A
ATOM       13   N   ASP A   4     29.172   6.115  10.170  1.00 28.70       A
ATOM       14   CA  ASP A   4     29.173   7.416  10.822  1.00 26.95       A
ATOM       15   CB  ASP A   4     27.812   7.722  11.456  1.00 28.65       A
ATOM       16   CG  ASP A   4     26.687   7.845  10.431  1.00 31.67       A
ATOM       17   OD1 ASP A   4     26.904   8.417   9.339  1.00 33.31       A
ATOM       18   OD2 ASP A   4     25.568   7.381  10.735  1.00 33.31       A
ATOM       19   C   ASP A   4     30.254   7.432  11.898  1.00 26.51       A
ATOM       20   O   ASP A   4     30.857   8.469  12.170  1.00 25.25       A
ATOM       21   N   HIS A   5     30.493   6.277  12.515  1.00 26.22       A
ATOM       22   CA  HIS A   5     31.527   6.164  13.544  1.00 26.52       A
ATOM       23   CB  HIS A   5     30.939   6.339  14.950  1.00 25.34       A
ATOM       24   CG  HIS A   5     30.240   7.647  15.156  1.00 28.69       A
ATOM       25   CD2 HIS A   5     30.716   8.870  15.492  1.00 29.15       A
ATOM       26   ND1 HIS A   5     28.881   7.801  14.979  1.00 28.23       A
ATOM       27   CE1 HIS A   5     28.550   9.062  15.198  1.00 29.92       A
ATOM       28   NE2 HIS A   5     29.645   9.732  15.511  1.00 29.84       A
ATOM       29   C   HIS A   5     32.246   4.826  13.465  1.00 25.79       A
ATOM       30   O   HIS A   5     31.630   3.785  13.227  1.00 25.68       A
ATOM       31   N   VAL A   6     33.559   4.866  13.659  1.00 24.52       A
ATOM       32   CA  VAL A   6     34.385   3.667  13.628  1.00 23.27       A
ATOM       33   CB  VAL A   6     35.311   3.657  12.407  1.00 25.22       A
ATOM       34   CG1 VAL A   6     36.187   2.414  12.440  1.00 24.31       A
ATOM       35   CG2 VAL A   6     34.489   3.708  11.127  1.00 27.15       A
ATOM       36   C   VAL A   6     35.256   3.633  14.876  1.00 22.15       A
ATOM       37   O   VAL A   6     35.937   4.606  15.185  1.00 21.49       A
ATOM       38   N   ALA A   7     35.239   2.513  15.586  1.00 19.90       A
ATOM       39   CA  ALA A   7     36.038   2.382  16.799  1.00 19.70       A
ATOM       40   CB  ALA A   7     35.132   2.394  18.034  1.00 14.59       A
ATOM       41   C   ALA A   7     36.867   1.111  16.791  1.00 18.62       A
ATOM       42   O   ALA A   7     36.548   0.153  16.088  1.00 20.78       A
ATOM       43   N   SER A   8     37.947   1.120  17.560  1.00 16.95       A
ATOM       44   CA  SER A   8     38.807  -0.048  17.700  1.00 18.62       A
ATOM       45   CB  SER A   8     40.211   0.215  17.153  1.00 17.69       A
ATOM       46   OG  SER A   8     40.209   0.271  15.738  1.00 19.81       A
ATOM       47   C   SER A   8     38.868  -0.310  19.199  1.00 18.76       A
ATOM       48   O   SER A   8     39.570   0.376  19.943  1.00 19.35       A
ATOM       49   N   TYR A   9     38.070  -1.268  19.645  1.00 19.38       A
ATOM       50   CA  TYR A   9     38.038  -1.608  21.048  1.00 19.44       A
ATOM       51   CB  TYR A   9     36.628  -1.980  21.471  1.00 19.18       A
ATOM       52   CG  TYR A   9     35.714  -0.785  21.375  1.00 18.65       A
ATOM       53   CD1 TYR A   9     36.073   0.435  21.962  1.00 16.57       A
ATOM       54   CE1 TYR A   9     35.237   1.537  21.897  1.00 17.39       A
ATOM       55   CD2 TYR A   9     34.493  -0.865  20.716  1.00 17.15       A
ATOM       56   CE2 TYR A   9     33.641   0.235  20.647  1.00 16.82       A
ATOM       57   CZ  TYR A   9     34.020   1.431  21.243  1.00 18.07       A
ATOM       58   OH  TYR A   9     33.169   2.509  21.210  1.00 19.77       A
ATOM       59   C   TYR A   9     38.993  -2.751  21.106  1.00 20.21       A
ATOM       60   O   TYR A   9     38.652  -3.911  21.344  1.00 15.05       A
ATOM       61   N   GLY A  10     40.225  -2.357  20.831  1.00 21.69       A
ATOM       62   CA  GLY A  10     41.311  -3.275  20.808  1.00 22.54       A
ATOM       63   C   GLY A  10     42.276  -3.080  19.655  1.00 21.74       A
ATOM       64   O   GLY A  10     42.248  -3.863  18.713  1.00 22.02       A
ATOM       65   N   VAL A  11     43.083  -2.023  19.674  1.00 18.91       A
ATOM       66   CA  VAL A  11     44.119  -1.949  18.651  1.00 17.39       A
ATOM       67   CB  VAL A  11     44.554  -0.506  18.277  1.00 18.75       A
ATOM       68   CG1 VAL A  11     45.845  -0.558  17.455  1.00 16.18       A
ATOM       69   CG2 VAL A  11     43.481   0.165  17.432  1.00 15.25       A
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ATOM      70   C    VAL A   11      45.228   -2.644   19.447   1.00 17.05          A
ATOM      71   O    VAL A   11      45.679   -2.145   20.481   1.00 19.34          A
ATOM      72   N    ASN A   12      45.616   -3.828   19.005   1.00 17.39          A
ATOM      73   CA   ASN A   12      46.643   -4.597   19.693   1.00 17.18          A
ATOM      74   CB   ASN A   12      46.113   -5.994   20.052   1.00 15.04          A
ATOM      75   CG   ASN A   12      44.834   -5.947   20.882   1.00 15.96          A
ATOM      76   OD1  ASN A   12      43.780   -5.490   20.417   1.00 18.20          A
ATOM      77   ND2  ASN A   12      44.921   -6.420   22.114   1.00 10.46          A
ATOM      78   C    ASN A   12      47.863   -4.739   18.797   1.00 18.90          A
ATOM      79   O    ASN A   12      47.752   -5.162   17.641   1.00 18.80          A
ATOM      80   N    LEU A   13      49.026   -4.403   19.343   1.00 18.60          A
ATOM      81   CA   LEU A   13      50.264   -4.478   18.599   1.00 19.90          A
ATOM      82   CB   LEU A   13      50.695   -3.064   18.217   1.00 23.26          A
ATOM      83   CG   LEU A   13      52.077   -2.881   17.594   1.00 24.86          A
ATOM      84   CD1  LEU A   13      52.085   -3.494   16.201   1.00 26.92          A
ATOM      85   CD2  LEU A   13      52.417   -1.402   17.534   1.00 24.75          A
ATOM      86   C    LEU A   13      51.391   -5.165   19.370   1.00 20.37          A
ATOM      87   O    LEU A   13      51.559   -4.953   20.566   1.00 21.11          A
ATOM      88   N    TYR A   14      52.145   -6.004   18.673   1.00 21.04          A
ATOM      89   CA   TYR A   14      53.291   -6.691   19.255   1.00 24.07          A
ATOM      90   CB   TYR A   14      52.909   -8.050   19.844   1.00 27.05          A
ATOM      91   CG   TYR A   14      54.091   -8.729   20.489   1.00 29.27          A
ATOM      92   CD1  TYR A   14      54.569   -8.304   21.723   1.00 30.07          A
ATOM      93   CE1  TYR A   14      55.709   -8.867   22.285   1.00 31.38          A
ATOM      94   CD2  TYR A   14      54.783   -9.744   19.830   1.00 31.63          A
ATOM      95   CE2  TYR A   14      55.923  -10.314   20.383   1.00 30.29          A
ATOM      96   CZ   TYR A   14      56.381   -9.868   21.609   1.00 31.37          A
ATOM      97   OH   TYR A   14      57.515  -10.413   22.160   1.00 34.48          A
ATOM      98   C    TYR A   14      54.291   -6.900   18.128   1.00 25.30          A
ATOM      99   O    TYR A   14      53.907   -7.206   16.994   1.00 25.51          A
ATOM     100   N    GLN A   15      55.571   -6.725   18.429   1.00 24.61          A
ATOM     101   CA   GLN A   15      56.603   -6.891   17.414   1.00 25.19          A
ATOM     102   CB   GLN A   15      56.932   -5.549   16.754   1.00 23.54          A
ATOM     103   CG   GLN A   15      57.278   -4.443   17.738   1.00 23.98          A
ATOM     104   CD   GLN A   15      57.567   -3.116   17.056   1.00 26.32          A
ATOM     105   OE1  GLN A   15      57.575   -2.062   17.702   1.00 28.26          A
ATOM     106   NE2  GLN A   15      57.810   -3.159   15.749   1.00 24.64          A
ATOM     107   C    GLN A   15      57.848   -7.487   18.036   1.00 26.16          A
ATOM     108   O    GLN A   15      58.134   -7.263   19.211   1.00 24.31          A
ATOM     109   N    SER A   16      58.583   -8.252   17.236   1.00 28.72          A
ATOM     110   CA   SER A   16      59.801   -8.912   17.698   1.00 30.37          A
ATOM     111   CB   SER A   16      60.341   -9.830   16.603   1.00 28.35          A
ATOM     112   OG   SER A   16      60.569   -9.100   15.407   1.00 31.43          A
ATOM     113   C    SER A   16      60.883   -7.918   18.111   1.00 32.37          A
ATOM     114   O    SER A   16      61.538   -8.104   19.134   1.00 33.91          A
ATOM     115   N    TYR A   17      61.073   -6.863   17.325   1.00 32.49          A
ATOM     116   CA   TYR A   17      62.096   -5.890   17.664   1.00 34.27          A
ATOM     117   CB   TYR A   17      62.172   -4.788   16.620   1.00 35.41          A
ATOM     118   CG   TYR A   17      63.371   -3.911   16.837   1.00 37.77          A
ATOM     119   CD1  TYR A   17      64.646   -4.347   16.470   1.00 39.38          A
ATOM     120   CE1  TYR A   17      65.769   -3.569   16.715   1.00 40.15          A
ATOM     121   CD2  TYR A   17      63.247   -2.671   17.456   1.00 36.31          A
ATOM     122   CE2  TYR A   17      64.360   -1.886   17.707   1.00 39.40          A
ATOM     123   CZ   TYR A   17      65.621   -2.338   17.335   1.00 41.42          A
ATOM     124   OH   TYR A   17      66.732   -1.562   17.580   1.00 43.02          A
ATOM     125   C    TYR A   17      61.821   -5.270   19.027   1.00 34.43          A
ATOM     126   O    TYR A   17      60.765   -4.682   19.248   1.00 35.58          A
ATOM     127   N    GLY A   18      62.783   -5.390   19.935   1.00 34.98          A
ATOM     128   CA   GLY A   18      62.609   -4.854   21.270   1.00 35.78          A
ATOM     129   C    GLY A   18      62.730   -5.968   22.292   1.00 36.87          A
ATOM     130   O    GLY A   18      63.761   -6.082   22.952   1.00 38.48          A
ATOM     131   N    PRO A   19      61.692   -6.807   22.459   1.00 37.06          A
ATOM     132   CD   PRO A   19      61.745   -7.967   23.368   1.00 35.58          A
ATOM     133   CA   PRO A   19      60.409   -6.769   21.747   1.00 34.79          A
ATOM     134   CB   PRO A   19      59.853   -8.166   21.981   1.00 35.91          A
ATOM     135   CG   PRO A   19      60.300   -8.437   23.394   1.00 36.88          A
ATOM     136   C    PRO A   19      59.531   -5.706   22.379   1.00 33.10          A
ATOM     137   O    PRO A   19      59.844   -5.209   23.456   1.00 33.71          A
ATOM     138   N    SER A   20      58.435   -5.349   21.722   1.00 31.83          A
ATOM     139   CA   SER A   20      57.548   -4.341   22.290   1.00 30.25          A
ATOM     140   CB   SER A   20      58.060   -2.932   21.965   1.00 29.00          A
ATOM     141   OG   SER A   20      58.072   -2.689   20.567   1.00 32.27          A
ATOM     142   C    SER A   20      56.108   -4.497   21.820   1.00 27.93          A
ATOM     143   O    SER A   20      55.829   -5.129   20.805   1.00 28.23          A
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| ATOM | 144 | N | GLY A | 21 | 55.191 | -3.911 | 22.576 | 1.00 | 25.87 | A |
|------|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| ATOM | 145 | CA | GLY A | 21 | 53.797 | -4.001 | 22.222 | 1.00 | 23.78 | A |
| ATOM | 146 | C | GLY A | 21 | 53.076 | -2.732 | 22.598 | 1.00 | 23.94 | A |
| ATOM | 147 | O | GLY A | 21 | 53.638 | -1.840 | 23.247 | 1.00 | 24.81 | A |
| ATOM | 148 | N | GLN A | 22 | 51.821 | -2.641 | 22.187 | 1.00 | 20.60 | A |
| ATOM | 149 | CA | GLN A | 22 | 51.033 | -1.470 | 22.495 | 1.00 | 19.67 | A |
| ATOM | 150 | CB | GLN A | 22 | 51.239 | -0.400 | 21.415 | 1.00 | 19.28 | A |
| ATOM | 151 | CG | GLN A | 22 | 50.584 | 0.943 | 21.736 | 1.00 | 18.12 | A |
| ATOM | 152 | CD | GLN A | 22 | 50.732 | 1.971 | 20.613 | 1.00 | 18.84 | A |
| ATOM | 153 | OE1 | GLN A | 22 | 51.694 | 2.749 | 20.576 | 1.00 | 19.77 | A |
| ATOM | 154 | NE2 | GLN A | 22 | 49.777 | 1.968 | 19.688 | 1.00 | 16.83 | A |
| ATOM | 155 | C | GLN A | 22 | 49.573 | -1.873 | 22.566 | 1.00 | 18.66 | A |
| ATOM | 156 | O | GLN A | 22 | 49.128 | -2.747 | 21.826 | 1.00 | 18.45 | A |
| ATOM | 157 | N | TYR A | 23 | 48.842 | -1.257 | 23.484 | 1.00 | 17.25 | A |
| ATOM | 158 | CA | TYR A | 23 | 47.423 | -1.529 | 23.615 | 1.00 | 16.53 | A |
| ATOM | 159 | CB | TYR A | 23 | 47.127 | -2.497 | 24.752 | 1.00 | 14.51 | A |
| ATOM | 160 | CG | TYR A | 23 | 45.674 | -2.904 | 24.760 | 1.00 | 12.67 | A |
| ATOM | 161 | CD1 | TYR A | 23 | 45.251 | -4.070 | 24.121 | 1.00 | 13.38 | A |
| ATOM | 162 | CE1 | TYR A | 23 | 43.904 | -4.415 | 24.070 | 1.00 | 13.23 | A |
| ATOM | 163 | CD2 | TYR A | 23 | 44.713 | -2.093 | 25.346 | 1.00 | 11.07 | A |
| ATOM | 164 | CE2 | TYR A | 23 | 43.365 | -2.425 | 25.299 | 1.00 | 12.99 | A |
| ATOM | 165 | CZ | TYR A | 23 | 42.964 | -3.583 | 24.664 | 1.00 | 13.72 | A |
| ATOM | 166 | OH | TYR A | 23 | 41.624 | -3.907 | 24.611 | 1.00 | 17.15 | A |
| ATOM | 167 | C | TYR A | 23 | 46.694 | -0.220 | 23.860 | 1.00 | 16.88 | A |
| ATOM | 168 | O | TYR A | 23 | 46.975 | 0.491 | 24.824 | 1.00 | 16.57 | A |
| ATOM | 169 | N | THR A | 24 | 45.757 | 0.085 | 22.969 | 1.00 | 16.16 | A |
| ATOM | 170 | CA | THR A | 24 | 44.975 | 1.311 | 23.038 | 1.00 | 16.43 | A |
| ATOM | 171 | CB | THR A | 24 | 45.594 | 2.405 | 22.136 | 1.00 | 18.41 | A |
| ATOM | 172 | OG1 | THR A | 24 | 45.581 | 1.954 | 20.771 | 1.00 | 17.20 | A |
| ATOM | 173 | CG2 | THR A | 24 | 47.029 | 2.692 | 22.537 | 1.00 | 18.64 | A |
| ATOM | 174 | C | THR A | 24 | 43.570 | 1.058 | 22.499 | 1.00 | 15.15 | A |
| ATOM | 175 | O | THR A | 24 | 43.314 | 0.037 | 21.879 | 1.00 | 15.70 | A |
| ATOM | 176 | N | HIS A | 25 | 42.667 | 1.993 | 22.754 | 1.00 | 15.66 | A |
| ATOM | 177 | CA | HIS A | 25 | 41.320 | 1.924 | 22.210 | 1.00 | 15.79 | A |
| ATOM | 178 | CB | HIS A | 25 | 40.243 | 1.834 | 23.297 | 1.00 | 13.55 | A |
| ATOM | 179 | CG | HIS A | 25 | 39.956 | 0.430 | 23.734 | 1.00 | 15.91 | A |
| ATOM | 180 | CD2 | HIS A | 25 | 40.688 | -0.704 | 23.624 | 1.00 | 13.86 | A |
| ATOM | 181 | ND1 | HIS A | 25 | 38.790 | 0.071 | 24.374 | 1.00 | 15.91 | A |
| ATOM | 182 | CE1 | HIS A | 25 | 38.815 | -1.222 | 24.639 | 1.00 | 14.38 | A |
| ATOM | 183 | NE2 | HIS A | 25 | 39.956 | -1.715 | 24.193 | 1.00 | 16.99 | A |
| ATOM | 184 | C | HIS A | 25 | 41.176 | 3.212 | 21.437 | 1.00 | 14.18 | A |
| ATOM | 185 | O | HIS A | 25 | 41.677 | 4.241 | 21.865 | 1.00 | 13.52 | A |
| ATOM | 186 | N | GLU A | 26 | 40.510 | 3.150 | 20.292 | 1.00 | 14.81 | A |
| ATOM | 187 | CA | GLU A | 26 | 40.333 | 4.329 | 19.462 | 1.00 | 16.96 | A |
| ATOM | 188 | CB | GLU A | 26 | 41.132 | 4.188 | 18.164 | 1.00 | 16.34 | A |
| ATOM | 189 | CG | GLU A | 26 | 42.644 | 4.158 | 18.311 | 1.00 | 18.80 | A |
| ATOM | 190 | CD | GLU A | 26 | 43.345 | 4.036 | 16.958 | 1.00 | 22.68 | A |
| ATOM | 191 | OE1 | GLU A | 26 | 42.744 | 4.456 | 15.946 | 1.00 | 26.77 | A |
| ATOM | 192 | OE2 | GLU A | 26 | 44.490 | 3.539 | 16.901 | 1.00 | 20.46 | A |
| ATOM | 193 | C | GLU A | 26 | 38.875 | 4.543 | 19.101 | 1.00 | 17.22 | A |
| ATOM | 194 | O | GLU A | 26 | 38.104 | 3.597 | 18.996 | 1.00 | 18.66 | A |
| ATOM | 195 | N | PHE A | 27 | 38.503 | 5.802 | 18.917 | 1.00 | 18.91 | A |
| ATOM | 196 | CA | PHE A | 27 | 37.150 | 6.135 | 18.509 | 1.00 | 19.32 | A |
| ATOM | 197 | CB | PHE A | 27 | 36.290 | 6.546 | 19.698 | 1.00 | 20.19 | A |
| ATOM | 198 | CG | PHE A | 27 | 34.834 | 6.653 | 19.357 | 1.00 | 23.33 | A |
| ATOM | 199 | CD1 | PHE A | 27 | 34.024 | 5.524 | 19.360 | 1.00 | 22.07 | A |
| ATOM | 200 | CD2 | PHE A | 27 | 34.289 | 7.868 | 18.971 | 1.00 | 23.24 | A |
| ATOM | 201 | CE1 | PHE A | 27 | 32.692 | 5.606 | 18.980 | 1.00 | 26.16 | A |
| ATOM | 202 | CE2 | PHE A | 27 | 32.954 | 7.962 | 18.587 | 1.00 | 25.99 | A |
| ATOM | 203 | CZ | PHE A | 27 | 32.155 | 6.828 | 18.592 | 1.00 | 25.46 | A |
| ATOM | 204 | C | PHE A | 27 | 37.260 | 7.291 | 17.522 | 1.00 | 19.10 | A |
| ATOM | 205 | O | PHE A | 27 | 37.733 | 8.375 | 17.871 | 1.00 | 19.83 | A |
| ATOM | 206 | N | ASP A | 28 | 36.831 | 7.052 | 16.288 | 1.00 | 19.17 | A |
| ATOM | 207 | CA | ASP A | 28 | 36.901 | 8.060 | 15.227 | 1.00 | 18.94 | A |
| ATOM | 208 | CB | ASP A | 28 | 35.910 | 9.203 | 15.473 | 1.00 | 21.33 | A |
| ATOM | 209 | CG | ASP A | 28 | 34.472 | 8.787 | 15.223 | 1.00 | 24.96 | A |
| ATOM | 210 | OD1 | ASP A | 28 | 34.266 | 7.801 | 14.484 | 1.00 | 25.18 | A |
| ATOM | 211 | OD2 | ASP A | 28 | 33.552 | 9.448 | 15.749 | 1.00 | 27.42 | A |
| ATOM | 212 | C | ASP A | 28 | 38.297 | 8.640 | 15.043 | 1.00 | 17.57 | A |
| ATOM | 213 | O | ASP A | 28 | 38.467 | 9.853 | 14.955 | 1.00 | 17.04 | A |
| ATOM | 214 | N | GLY A | 29 | 39.292 | 7.760 | 15.002 | 1.00 | 17.53 | A |
| ATOM | 215 | CA | GLY A | 29 | 40.658 | 8.189 | 14.779 | 1.00 | 17.51 | A |
| ATOM | 216 | C | GLY A | 29 | 41.437 | 8.738 | 15.953 | 1.00 | 16.95 | A |
| ATOM | 217 | O | GLY A | 29 | 42.621 | 9.010 | 15.814 | 1.00 | 19.26 | A |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 218 | N | ASP | A | 30 | 40.797 | 8.922 | 17.098 | 1.00 16.92 | A |
| ATOM | 219 | CA | ASP | A | 30 | 41.511 | 9.438 | 18.254 | 1.00 16.83 | A |
| ATOM | 220 | CB | ASP | A | 30 | 40.816 | 10.678 | 18.796 | 1.00 18.99 | A |
| ATOM | 221 | CG | ASP | A | 30 | 40.988 | 11.864 | 17.888 | 1.00 21.09 | A |
| ATOM | 222 | OD1 | ASP | A | 30 | 42.145 | 12.177 | 17.538 | 1.00 22.94 | A |
| ATOM | 223 | OD2 | ASP | A | 30 | 39.971 | 12.478 | 17.525 | 1.00 21.68 | A |
| ATOM | 224 | C | ASP | A | 30 | 41.656 | 8.392 | 19.345 | 1.00 17.25 | A |
| ATOM | 225 | O | ASP | A | 30 | 40.777 | 7.553 | 19.543 | 1.00 15.40 | A |
| ATOM | 226 | N | GLU | A | 31 | 42.784 | 8.453 | 20.041 | 1.00 16.77 | A |
| ATOM | 227 | CA | GLU | A | 31 | 43.111 | 7.514 | 21.107 | 1.00 18.43 | A |
| ATOM | 228 | CB | GLU | A | 31 | 44.620 | 7.607 | 21.392 | 1.00 20.90 | A |
| ATOM | 229 | CG | GLU | A | 31 | 45.147 | 6.853 | 22.608 | 1.00 24.68 | A |
| ATOM | 230 | CD | GLU | A | 31 | 46.678 | 6.924 | 22.702 | 1.00 27.25 | A |
| ATOM | 231 | OE1 | GLU | A | 31 | 47.258 | 7.931 | 22.239 | 1.00 26.93 | A |
| ATOM | 232 | OE2 | GLU | A | 31 | 47.302 | 5.985 | 23.242 | 1.00 27.21 | A |
| ATOM | 233 | C | GLU | A | 31 | 42.296 | 7.777 | 22.375 | 1.00 17.51 | A |
| ATOM | 234 | O | GLU | A | 31 | 42.361 | 8.863 | 22.952 | 1.00 17.13 | A |
| ATOM | 235 | N | GLN | A | 32 | 41.525 | 6.784 | 22.807 | 1.00 15.52 | A |
| ATOM | 236 | CA | GLN | A | 32 | 40.726 | 6.942 | 24.020 | 1.00 16.47 | A |
| ATOM | 237 | CB | GLN | A | 32 | 39.542 | 5.980 | 24.009 | 1.00 15.91 | A |
| ATOM | 238 | CG | GLN | A | 32 | 38.439 | 6.399 | 23.065 | 1.00 15.97 | A |
| ATOM | 239 | CD | GLN | A | 32 | 37.292 | 5.419 | 23.071 | 1.00 20.20 | A |
| ATOM | 240 | OE1 | GLN | A | 32 | 37.478 | 4.228 | 22.808 | 1.00 18.09 | A |
| ATOM | 241 | NE2 | GLN | A | 32 | 36.091 | 5.912 | 23.374 | 1.00 20.57 | A |
| ATOM | 242 | C | GLN | A | 32 | 41.584 | 6.701 | 25.255 | 1.00 16.61 | A |
| ATOM | 243 | O | GLN | A | 32 | 41.448 | 7.387 | 26.272 | 1.00 15.51 | A |
| ATOM | 244 | N | PHE | A | 33 | 42.470 | 5.720 | 25.151 | 1.00 15.59 | A |
| ATOM | 245 | CA | PHE | A | 33 | 43.370 | 5.389 | 26.239 | 1.00 16.34 | A |
| ATOM | 246 | CB | PHE | A | 33 | 42.583 | 4.854 | 27.443 | 1.00 17.21 | A |
| ATOM | 247 | CG | PHE | A | 33 | 41.951 | 3.502 | 27.222 | 1.00 16.68 | A |
| ATOM | 248 | CD1 | PHE | A | 33 | 42.686 | 2.333 | 27.406 | 1.00 15.57 | A |
| ATOM | 249 | CD2 | PHE | A | 33 | 40.598 | 3.397 | 26.903 | 1.00 18.54 | A |
| ATOM | 250 | CE1 | PHE | A | 33 | 42.083 | 1.076 | 27.288 | 1.00 16.34 | A |
| ATOM | 251 | CE2 | PHE | A | 33 | 39.983 | 2.147 | 26.782 | 1.00 17.35 | A |
| ATOM | 252 | CZ | PHE | A | 33 | 40.729 | 0.983 | 26.978 | 1.00 16.56 | A |
| ATOM | 253 | C | PHE | A | 33 | 44.363 | 4.343 | 25.776 | 1.00 16.66 | A |
| ATOM | 254 | O | PHE | A | 33 | 44.209 | 3.746 | 24.712 | 1.00 16.85 | A |
| ATOM | 255 | N | TYR | A | 34 | 45.398 | 4.139 | 26.572 | 1.00 16.03 | A |
| ATOM | 256 | CA | TYR | A | 34 | 46.377 | 3.125 | 26.264 | 1.00 16.93 | A |
| ATOM | 257 | CB | TYR | A | 34 | 47.636 | 3.730 | 25.621 | 1.00 16.33 | A |
| ATOM | 258 | CG | TYR | A | 34 | 48.528 | 4.541 | 26.523 | 1.00 17.31 | A |
| ATOM | 259 | CD1 | TYR | A | 34 | 49.519 | 3.930 | 27.291 | 1.00 17.48 | A |
| ATOM | 260 | CE1 | TYR | A | 34 | 50.367 | 4.683 | 28.097 | 1.00 19.16 | A |
| ATOM | 261 | CD2 | TYR | A | 34 | 48.404 | 5.928 | 26.586 | 1.00 17.68 | A |
| ATOM | 262 | CE2 | TYR | A | 34 | 49.244 | 6.690 | 27.388 | 1.00 19.73 | A |
| ATOM | 263 | CZ | TYR | A | 34 | 50.224 | 6.060 | 28.141 | 1.00 20.10 | A |
| ATOM | 264 | OH | TYR | A | 34 | 51.044 | 6.815 | 28.941 | 1.00 23.02 | A |
| ATOM | 265 | C | TYR | A | 34 | 46.692 | 2.473 | 27.588 | 1.00 17.88 | A |
| ATOM | 266 | O | TYR | A | 34 | 46.429 | 3.042 | 28.646 | 1.00 21.13 | A |
| ATOM | 267 | N | VAL | A | 35 | 47.213 | 1.261 | 27.535 | 1.00 17.31 | A |
| ATOM | 268 | CA | VAL | A | 35 | 47.571 | 0.570 | 28.749 | 1.00 18.89 | A |
| ATOM | 269 | CB | VAL | A | 35 | 46.950 | -0.848 | 28.804 | 1.00 19.12 | A |
| ATOM | 270 | CG1 | VAL | A | 35 | 47.589 | -1.660 | 29.912 | 1.00 17.56 | A |
| ATOM | 271 | CG2 | VAL | A | 35 | 45.454 | -0.742 | 29.048 | 1.00 19.75 | A |
| ATOM | 272 | C | VAL | A | 35 | 49.084 | 0.478 | 28.786 | 1.00 18.84 | A |
| ATOM | 273 | O | VAL | A | 35 | 49.701 | -0.050 | 27.877 | 1.00 16.51 | A |
| ATOM | 274 | N | ASP | A | 36 | 49.676 | 1.039 | 29.830 | 1.00 22.55 | A |
| ATOM | 275 | CA | ASP | A | 36 | 51.121 | 0.984 | 29.996 | 1.00 25.86 | A |
| ATOM | 276 | CB | ASP | A | 36 | 51.542 | 1.872 | 31.172 | 1.00 26.89 | A |
| ATOM | 277 | CG | ASP | A | 36 | 53.033 | 2.108 | 31.221 | 1.00 26.55 | A |
| ATOM | 278 | OD1 | ASP | A | 36 | 53.796 | 1.125 | 31.270 | 1.00 29.78 | A |
| ATOM | 279 | OD2 | ASP | A | 36 | 53.441 | 3.285 | 31.213 | 1.00 30.03 | A |
| ATOM | 280 | C | ASP | A | 36 | 51.393 | -0.484 | 30.314 | 1.00 26.39 | A |
| ATOM | 281 | O | ASP | A | 36 | 51.016 | -0.976 | 31.378 | 1.00 27.38 | A |
| ATOM | 282 | N | LEU | A | 37 | 52.024 | -1.187 | 29.387 | 1.00 27.51 | A |
| ATOM | 283 | CA | LEU | A | 37 | 52.305 | -2.600 | 29.588 | 1.00 29.51 | A |
| ATOM | 284 | CB | LEU | A | 37 | 52.754 | -3.231 | 28.270 | 1.00 26.29 | A |
| ATOM | 285 | CG | LEU | A | 37 | 51.704 | -3.111 | 27.160 | 1.00 25.10 | A |
| ATOM | 286 | CD1 | LEU | A | 37 | 52.265 | -3.630 | 25.852 | 1.00 21.32 | A |
| ATOM | 287 | CD2 | LEU | A | 37 | 50.455 | -3.876 | 27.557 | 1.00 22.51 | A |
| ATOM | 288 | C | LEU | A | 37 | 53.348 | -2.838 | 30.674 | 1.00 30.95 | A |
| ATOM | 289 | O | LEU | A | 37 | 53.222 | -3.774 | 31.457 | 1.00 31.43 | A |
| ATOM | 290 | N | GLY | A | 38 | 54.362 | -1.980 | 30.734 | 1.00 33.46 | A |
| ATOM | 291 | CA | GLY | A | 38 | 55.403 | -2.140 | 31.737 | 1.00 35.44 | A |

| ATOM | 292 | C   | GLY A | 38 | 54.956 | -1.863 | 33.162 | 1.00 | 37.63 | A |
|------|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| ATOM | 293 | O   | GLY A | 38 | 55.369 | -2.549 | 34.098 | 1.00 | 38.42 | A |
| ATOM | 294 | N   | ARG A | 39 | 54.101 | -0.861 | 33.334 | 1.00 | 38.93 | A |
| ATOM | 295 | CA  | ARG A | 39 | 53.625 | -0.499 | 34.660 | 1.00 | 40.81 | A |
| ATOM | 296 | CB  | ARG A | 39 | 53.645 | 1.029  | 34.803 | 1.00 | 42.41 | A |
| ATOM | 297 | CG  | ARG A | 39 | 54.968 | 1.627  | 34.339 | 1.00 | 44.76 | A |
| ATOM | 298 | CD  | ARG A | 39 | 55.113 | 3.118  | 34.619 | 1.00 | 47.83 | A |
| ATOM | 299 | NE  | ARG A | 39 | 56.318 | 3.644  | 33.976 | 1.00 | 50.52 | A |
| ATOM | 300 | CZ  | ARG A | 39 | 56.902 | 4.799  | 34.281 | 1.00 | 53.40 | A |
| ATOM | 301 | NH1 | ARG A | 39 | 56.399 | 5.575  | 35.235 | 1.00 | 54.01 | A |
| ATOM | 302 | NH2 | ARG A | 39 | 57.998 | 5.179  | 33.633 | 1.00 | 54.18 | A |
| ATOM | 303 | C   | ARG A | 39 | 52.229 | -1.057 | 34.936 | 1.00 | 41.12 | A |
| ATOM | 304 | O   | ARG A | 39 | 51.664 | -0.847 | 36.014 | 1.00 | 39.71 | A |
| ATOM | 305 | N   | LYS A | 40 | 51.687 | -1.779 | 33.955 | 1.00 | 40.65 | A |
| ATOM | 306 | CA  | LYS A | 40 | 50.365 | -2.380 | 34.070 | 1.00 | 39.55 | A |
| ATOM | 307 | CB  | LYS A | 40 | 50.415 | -3.554 | 35.053 | 1.00 | 42.42 | A |
| ATOM | 308 | CG  | LYS A | 40 | 49.196 | -4.467 | 34.996 | 1.00 | 46.46 | A |
| ATOM | 309 | CD  | LYS A | 40 | 49.266 | -5.563 | 36.054 | 1.00 | 50.42 | A |
| ATOM | 310 | CE  | LYS A | 40 | 48.077 | -6.513 | 35.947 | 1.00 | 51.25 | A |
| ATOM | 311 | NZ  | LYS A | 40 | 46.781 | -5.779 | 35.970 | 1.00 | 52.15 | A |
| ATOM | 312 | C   | LYS A | 40 | 49.338 | -1.348 | 34.540 | 1.00 | 37.45 | A |
| ATOM | 313 | O   | LYS A | 40 | 48.647 | -1.560 | 35.533 | 1.00 | 35.78 | A |
| ATOM | 314 | N   | GLU A | 41 | 49.245 | -0.237 | 33.812 | 1.00 | 35.81 | A |
| ATOM | 315 | CA  | GLU A | 41 | 48.317 | 0.847  | 34.142 | 1.00 | 33.83 | A |
| ATOM | 316 | CB  | GLU A | 41 | 49.077 | 2.079  | 34.655 | 1.00 | 36.46 | A |
| ATOM | 317 | CG  | GLU A | 41 | 49.660 | 1.997  | 36.049 | 1.00 | 41.33 | A |
| ATOM | 318 | CD  | GLU A | 41 | 50.500 | 3.224  | 36.374 | 1.00 | 44.23 | A |
| ATOM | 319 | OE1 | GLU A | 41 | 50.067 | 4.343  | 36.022 | 1.00 | 46.67 | A |
| ATOM | 320 | OE2 | GLU A | 41 | 51.585 | 3.076  | 36.981 | 1.00 | 45.55 | A |
| ATOM | 321 | C   | GLU A | 41 | 47.492 | 1.301  | 32.937 | 1.00 | 30.89 | A |
| ATOM | 322 | O   | GLU A | 41 | 47.995 | 1.373  | 31.816 | 1.00 | 27.89 | A |
| ATOM | 323 | N   | THR A | 42 | 46.227 | 1.623  | 33.182 | 1.00 | 28.11 | A |
| ATOM | 324 | CA  | THR A | 42 | 45.354 | 2.127  | 32.135 | 1.00 | 26.58 | A |
| ATOM | 325 | CB  | THR A | 42 | 43.882 | 1.773  | 32.406 | 1.00 | 27.67 | A |
| ATOM | 326 | OG1 | THR A | 42 | 43.716 | 0.349  | 32.394 | 1.00 | 25.55 | A |
| ATOM | 327 | CG2 | THR A | 42 | 42.979 | 2.419  | 31.357 | 1.00 | 25.33 | A |
| ATOM | 328 | C   | THR A | 42 | 45.506 | 3.642  | 32.212 | 1.00 | 26.90 | A |
| ATOM | 329 | O   | THR A | 42 | 45.305 | 4.232  | 33.269 | 1.00 | 25.79 | A |
| ATOM | 330 | N   | VAL A | 43 | 45.881 | 4.273  | 31.108 | 1.00 | 25.87 | A |
| ATOM | 331 | CA  | VAL A | 43 | 46.045 | 5.720  | 31.106 | 1.00 | 24.36 | A |
| ATOM | 332 | CB  | VAL A | 43 | 47.474 | 6.119  | 30.670 | 1.00 | 24.45 | A |
| ATOM | 333 | CG1 | VAL A | 43 | 47.698 | 7.606  | 30.906 | 1.00 | 24.38 | A |
| ATOM | 334 | CG2 | VAL A | 43 | 48.504 | 5.289  | 31.433 | 1.00 | 22.82 | A |
| ATOM | 335 | C   | VAL A | 43 | 45.039 | 6.331  | 30.141 | 1.00 | 24.94 | A |
| ATOM | 336 | O   | VAL A | 43 | 45.143 | 6.133  | 28.930 | 1.00 | 24.72 | A |
| ATOM | 337 | N   | TRP A | 44 | 44.063 | 7.065  | 30.672 | 1.00 | 24.50 | A |
| ATOM | 338 | CA  | TRP A | 44 | 43.050 | 7.681  | 29.824 | 1.00 | 25.64 | A |
| ATOM | 339 | CB  | TRP A | 44 | 41.804 | 8.033  | 30.642 | 1.00 | 25.03 | A |
| ATOM | 340 | CG  | TRP A | 44 | 41.224 | 6.859  | 31.370 | 1.00 | 25.96 | A |
| ATOM | 341 | CD2 | TRP A | 44 | 40.281 | 5.906  | 30.858 | 1.00 | 25.77 | A |
| ATOM | 342 | CE2 | TRP A | 44 | 40.067 | 4.946  | 31.870 | 1.00 | 26.64 | A |
| ATOM | 343 | CE3 | TRP A | 44 | 39.599 | 5.766  | 29.641 | 1.00 | 24.94 | A |
| ATOM | 344 | CD1 | TRP A | 44 | 41.529 | 6.450  | 32.634 | 1.00 | 26.43 | A |
| ATOM | 345 | NE1 | TRP A | 44 | 40.840 | 5.305  | 32.942 | 1.00 | 26.28 | A |
| ATOM | 346 | CZ2 | TRP A | 44 | 39.197 | 3.860  | 31.704 | 1.00 | 25.00 | A |
| ATOM | 347 | CZ3 | TRP A | 44 | 38.734 | 4.688  | 29.476 | 1.00 | 22.40 | A |
| ATOM | 348 | CH2 | TRP A | 44 | 38.542 | 3.749  | 30.501 | 1.00 | 24.18 | A |
| ATOM | 349 | C   | TRP A | 44 | 43.578 | 8.925  | 29.116 | 1.00 | 26.30 | A |
| ATOM | 350 | O   | TRP A | 44 | 44.321 | 9.713  | 29.700 | 1.00 | 24.42 | A |
| ATOM | 351 | N   | CYS A | 45 | 43.193 | 9.090  | 27.853 | 1.00 | 28.01 | A |
| ATOM | 352 | CA  | CYS A | 45 | 43.635 | 10.234 | 27.062 | 1.00 | 30.22 | A |
| ATOM | 353 | CB  | CYS A | 45 | 44.069 | 9.777  | 25.666 | 1.00 | 29.51 | A |
| ATOM | 354 | SG  | CYS A | 45 | 45.547 | 8.727  | 25.680 | 1.00 | 30.66 | A |
| ATOM | 355 | C   | CYS A | 45 | 42.574 | 11.317 | 26.951 | 1.00 | 31.06 | A |
| ATOM | 356 | O   | CYS A | 45 | 42.836 | 12.399 | 26.428 | 1.00 | 34.14 | A |
| ATOM | 357 | N   | LEU A | 46 | 41.375 | 11.016 | 27.439 | 1.00 | 31.99 | A |
| ATOM | 358 | CA  | LEU A | 46 | 40.261 | 11.965 | 27.436 | 1.00 | 32.61 | A |
| ATOM | 359 | CB  | LEU A | 46 | 39.137 | 11.493 | 26.506 | 1.00 | 31.72 | A |
| ATOM | 360 | CG  | LEU A | 46 | 38.810 | 12.325 | 25.263 | 1.00 | 32.47 | A |
| ATOM | 361 | CD1 | LEU A | 46 | 37.492 | 11.830 | 24.674 | 1.00 | 28.87 | A |
| ATOM | 362 | CD2 | LEU A | 46 | 38.710 | 13.810 | 25.617 | 1.00 | 29.99 | A |
| ATOM | 363 | C   | LEU A | 46 | 39.734 | 12.042 | 28.869 | 1.00 | 32.81 | A |
| ATOM | 364 | O   | LEU A | 46 | 39.195 | 11.066 | 29.395 | 1.00 | 33.99 | A |
| ATOM | 365 | N   | PRO A | 47 | 39.893 | 13.201 | 29.521 | 1.00 | 32.52 | A |

| ATOM | 366 | CD | PRO A | 47 | 40.488 | 14.442 | 28.986 | 1.00 | 32.23 | A |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 367 | CA | PRO A | 47 | 39.437 | 13.392 | 30.901 | 1.00 | 32.18 | A |
| ATOM | 368 | CB | PRO A | 47 | 39.487 | 14.908 | 31.063 | 1.00 | 32.11 | A |
| ATOM | 369 | CG | PRO A | 47 | 40.690 | 15.270 | 30.236 | 1.00 | 31.60 | A |
| ATOM | 370 | C | PRO A | 47 | 38.066 | 12.800 | 31.245 | 1.00 | 30.96 | A |
| ATOM | 371 | O | PRO A | 47 | 37.927 | 12.103 | 32.243 | 1.00 | 30.17 | A |
| ATOM | 372 | N | VAL A | 48 | 37.064 | 13.068 | 30.418 | 1.00 | 30.75 | A |
| ATOM | 373 | CA | VAL A | 48 | 35.715 | 12.563 | 30.663 | 1.00 | 32.56 | A |
| ATOM | 374 | CB | VAL A | 48 | 34.748 | 13.040 | 29.560 | 1.00 | 34.04 | A |
| ATOM | 375 | CG1 | VAL A | 48 | 33.320 | 12.683 | 29.932 | 1.00 | 34.16 | A |
| ATOM | 376 | CG2 | VAL A | 48 | 34.881 | 14.556 | 29.368 | 1.00 | 38.02 | A |
| ATOM | 377 | C | VAL A | 48 | 35.633 | 11.033 | 30.765 | 1.00 | 33.13 | A |
| ATOM | 378 | O | VAL A | 48 | 34.698 | 10.485 | 31.355 | 1.00 | 33.55 | A |
| ATOM | 379 | N | LEU A | 49 | 36.615 | 10.350 | 30.192 | 1.00 | 33.30 | A |
| ATOM | 380 | CA | LEU A | 49 | 36.661 | 8.892 | 30.208 | 1.00 | 32.44 | A |
| ATOM | 381 | CB | LEU A | 49 | 37.498 | 8.391 | 29.023 | 1.00 | 30.62 | A |
| ATOM | 382 | CG | LEU A | 49 | 36.792 | 8.027 | 27.702 | 1.00 | 31.64 | A |
| ATOM | 383 | CD1 | LEU A | 49 | 35.578 | 8.888 | 27.464 | 1.00 | 29.12 | A |
| ATOM | 384 | CD2 | LEU A | 49 | 37.783 | 8.157 | 26.551 | 1.00 | 31.05 | A |
| ATOM | 385 | C | LEU A | 49 | 37.226 | 8.343 | 31.519 | 1.00 | 33.77 | A |
| ATOM | 386 | O | LEU A | 49 | 37.138 | 7.142 | 31.787 | 1.00 | 34.14 | A |
| ATOM | 387 | N | ARG A | 50 | 37.794 | 9.221 | 32.339 | 1.00 | 34.56 | A |
| ATOM | 388 | CA | ARG A | 50 | 38.367 | 8.810 | 33.618 | 1.00 | 35.58 | A |
| ATOM | 389 | CB | ARG A | 50 | 38.987 | 10.009 | 34.345 | 1.00 | 37.99 | A |
| ATOM | 390 | CG | ARG A | 50 | 40.137 | 10.720 | 33.636 | 1.00 | 40.65 | A |
| ATOM | 391 | CD | ARG A | 50 | 40.657 | 11.846 | 34.529 | 1.00 | 43.05 | A |
| ATOM | 392 | NE | ARG A | 50 | 41.603 | 12.748 | 33.872 | 1.00 | 44.85 | A |
| ATOM | 393 | CZ | ARG A | 50 | 42.815 | 12.403 | 33.444 | 1.00 | 46.08 | A |
| ATOM | 394 | NH1 | ARG A | 50 | 43.254 | 11.159 | 33.592 | 1.00 | 46.76 | A |
| ATOM | 395 | NH2 | ARG A | 50 | 43.599 | 13.314 | 32.880 | 1.00 | 46.08 | A |
| ATOM | 396 | C | ARG A | 50 | 37.334 | 8.168 | 34.547 | 1.00 | 35.55 | A |
| ATOM | 397 | O | ARG A | 50 | 37.693 | 7.475 | 35.495 | 1.00 | 35.21 | A |
| ATOM | 398 | N | GLN A | 51 | 36.054 | 8.412 | 34.284 | 1.00 | 36.77 | A |
| ATOM | 399 | CA | GLN A | 51 | 34.987 | 7.859 | 35.116 | 1.00 | 37.34 | A |
| ATOM | 400 | CB | GLN A | 51 | 33.658 | 8.558 | 34.821 | 1.00 | 39.02 | A |
| ATOM | 401 | CG | GLN A | 51 | 33.123 | 8.306 | 33.418 | 1.00 | 41.24 | A |
| ATOM | 402 | CD | GLN A | 51 | 31.765 | 8.947 | 33.189 | 1.00 | 43.49 | A |
| ATOM | 403 | OE1 | GLN A | 51 | 30.781 | 8.597 | 33.843 | 1.00 | 43.80 | A |
| ATOM | 404 | NE2 | GLN A | 51 | 31.706 | 9.895 | 32.260 | 1.00 | 44.01 | A |
| ATOM | 405 | C | GLN A | 51 | 34.821 | 6.362 | 34.896 | 1.00 | 36.85 | A |
| ATOM | 406 | O | GLN A | 51 | 34.250 | 5.665 | 35.734 | 1.00 | 37.06 | A |
| ATOM | 407 | N | PHE A | 52 | 35.316 | 5.871 | 33.764 | 1.00 | 35.13 | A |
| ATOM | 408 | CA | PHE A | 52 | 35.218 | 4.454 | 33.446 | 1.00 | 32.82 | A |
| ATOM | 409 | CB | PHE A | 52 | 35.143 | 4.258 | 31.931 | 1.00 | 31.28 | A |
| ATOM | 410 | CG | PHE A | 52 | 33.902 | 4.838 | 31.301 | 1.00 | 29.86 | A |
| ATOM | 411 | CD1 | PHE A | 52 | 32.640 | 4.549 | 31.821 | 1.00 | 27.82 | A |
| ATOM | 412 | CD2 | PHE A | 52 | 33.992 | 5.652 | 30.177 | 1.00 | 27.71 | A |
| ATOM | 413 | CE1 | PHE A | 52 | 31.490 | 5.060 | 31.234 | 1.00 | 25.58 | A |
| ATOM | 414 | CE2 | PHE A | 52 | 32.847 | 6.171 | 29.580 | 1.00 | 28.10 | A |
| ATOM | 415 | CZ | PHE A | 52 | 31.592 | 5.873 | 30.111 | 1.00 | 28.21 | A |
| ATOM | 416 | C | PHE A | 52 | 36.405 | 3.675 | 34.004 | 1.00 | 32.57 | A |
| ATOM | 417 | O | PHE A | 52 | 37.370 | 4.256 | 34.494 | 1.00 | 32.22 | A |
| ATOM | 418 | N | ARG A | 53 | 36.327 | 2.353 | 33.927 | 1.00 | 32.80 | A |
| ATOM | 419 | CA | ARG A | 53 | 37.397 | 1.498 | 34.419 | 1.00 | 32.77 | A |
| ATOM | 420 | CB | ARG A | 53 | 37.005 | 0.862 | 35.760 | 1.00 | 36.56 | A |
| ATOM | 421 | CG | ARG A | 53 | 36.741 | 1.867 | 36.881 | 1.00 | 42.83 | A |
| ATOM | 422 | CD | ARG A | 53 | 36.523 | 1.168 | 38.214 | 1.00 | 49.04 | A |
| ATOM | 423 | NE | ARG A | 53 | 36.308 | 2.111 | 39.312 | 1.00 | 53.82 | A |
| ATOM | 424 | CZ | ARG A | 53 | 36.195 | 1.758 | 40.589 | 1.00 | 54.70 | A |
| ATOM | 425 | NH1 | ARG A | 53 | 36.277 | 0.478 | 40.937 | 1.00 | 55.50 | A |
| ATOM | 426 | NH2 | ARG A | 53 | 36.004 | 2.683 | 41.520 | 1.00 | 55.64 | A |
| ATOM | 427 | C | ARG A | 53 | 37.706 | 0.404 | 33.405 | 1.00 | 29.88 | A |
| ATOM | 428 | O | ARG A | 53 | 36.806 | -0.117 | 32.743 | 1.00 | 28.71 | A |
| ATOM | 429 | N | PHE A | 54 | 38.986 | 0.066 | 33.293 | 1.00 | 26.44 | A |
| ATOM | 430 | CA | PHE A | 54 | 39.440 | -0.960 | 32.371 | 1.00 | 22.47 | A |
| ATOM | 431 | CB | PHE A | 54 | 39.905 | -0.325 | 31.060 | 1.00 | 21.88 | A |
| ATOM | 432 | CG | PHE A | 54 | 40.181 | -1.320 | 29.974 | 1.00 | 20.69 | A |
| ATOM | 433 | CD1 | PHE A | 54 | 39.150 | -1.801 | 29.180 | 1.00 | 19.52 | A |
| ATOM | 434 | CD2 | PHE A | 54 | 41.471 | -1.782 | 29.750 | 1.00 | 18.68 | A |
| ATOM | 435 | CE1 | PHE A | 54 | 39.399 | -2.734 | 28.170 | 1.00 | 22.81 | A |
| ATOM | 436 | CE2 | PHE A | 54 | 41.733 | -2.714 | 28.746 | 1.00 | 20.58 | A |
| ATOM | 437 | CZ | PHE A | 54 | 40.697 | -3.190 | 27.954 | 1.00 | 20.86 | A |
| ATOM | 438 | C | PHE A | 54 | 40.597 | -1.711 | 33.017 | 1.00 | 23.43 | A |
| ATOM | 439 | O | PHE A | 54 | 41.631 | -1.122 | 33.351 | 1.00 | 23.53 | A |

| ATOM | 440 | N   | ASP | A | 55  | 40.408 | -3.011  | 33.198 | 1.00 | 22.82 | A |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 441 | CA  | ASP | A | 55  | 41.411 | -3.874  | 33.805 | 1.00 | 24.70 | A |
| ATOM | 442 | CB  | ASP | A | 55  | 40.785 | -5.246  | 34.083 | 1.00 | 23.26 | A |
| ATOM | 443 | CG  | ASP | A | 55  | 41.729 | -6.190  | 34.789 | 1.00 | 26.24 | A |
| ATOM | 444 | OD1 | ASP | A | 55  | 42.924 | -5.853  | 34.933 | 1.00 | 28.75 | A |
| ATOM | 445 | OD2 | ASP | A | 55  | 41.274 | -7.279  | 35.192 | 1.00 | 26.38 | A |
| ATOM | 446 | C   | ASP | A | 55  | 42.613 | -4.011  | 32.861 | 1.00 | 24.24 | A |
| ATOM | 447 | O   | ASP | A | 55  | 42.510 | -4.629  | 31.802 | 1.00 | 23.91 | A |
| ATOM | 448 | N   | PRO | A | 56  | 43.770 | -3.437  | 33.238 | 1.00 | 23.69 | A |
| ATOM | 449 | CD  | PRO | A | 56  | 44.084 | -2.761  | 34.509 | 1.00 | 23.79 | A |
| ATOM | 450 | CA  | PRO | A | 56  | 44.961 | -3.522  | 32.387 | 1.00 | 23.45 | A |
| ATOM | 451 | CB  | PRO | A | 56  | 46.002 | -2.707  | 33.162 | 1.00 | 23.35 | A |
| ATOM | 452 | CG  | PRO | A | 56  | 45.592 | -2.897  | 34.580 | 1.00 | 23.31 | A |
| ATOM | 453 | C   | PRO | A | 56  | 45.413 | -4.952  | 32.114 | 1.00 | 23.66 | A |
| ATOM | 454 | O   | PRO | A | 56  | 46.099 | -5.220  | 31.125 | 1.00 | 23.15 | A |
| ATOM | 455 | N   | GLN | A | 57  | 45.025 | -5.871  | 32.991 | 1.00 | 21.84 | A |
| ATOM | 456 | CA  | GLN | A | 57  | 45.397 | -7.261  | 32.818 | 1.00 | 22.47 | A |
| ATOM | 457 | CB  | GLN | A | 57  | 44.834 | -8.108  | 33.965 | 1.00 | 23.11 | A |
| ATOM | 458 | CG  | GLN | A | 57  | 45.226 | -9.568  | 33.873 | 1.00 | 20.82 | A |
| ATOM | 459 | CD  | GLN | A | 57  | 46.722 | -9.745  | 33.733 | 1.00 | 22.23 | A |
| ATOM | 460 | OE1 | GLN | A | 57  | 47.497 | -9.227  | 34.539 | 1.00 | 21.88 | A |
| ATOM | 461 | NE2 | GLN | A | 57  | 47.138 | -10.475 | 32.707 | 1.00 | 23.15 | A |
| ATOM | 462 | C   | GLN | A | 57  | 44.882 | -7.792  | 31.482 | 1.00 | 22.21 | A |
| ATOM | 463 | O   | GLN | A | 57  | 45.452 | -8.723  | 30.913 | 1.00 | 23.00 | A |
| ATOM | 464 | N   | PHE | A | 58  | 43.801 | -7.203  | 30.980 | 1.00 | 22.42 | A |
| ATOM | 465 | CA  | PHE | A | 58  | 43.254 | -7.640  | 29.704 | 1.00 | 21.07 | A |
| ATOM | 466 | CB  | PHE | A | 58  | 42.004 | -6.857  | 29.338 | 1.00 | 20.45 | A |
| ATOM | 467 | CG  | PHE | A | 58  | 41.411 | -7.287  | 28.031 | 1.00 | 21.03 | A |
| ATOM | 468 | CD1 | PHE | A | 58  | 40.472 | -8.312  | 27.988 | 1.00 | 18.42 | A |
| ATOM | 469 | CD2 | PHE | A | 58  | 41.864 | -6.736  | 26.835 | 1.00 | 18.79 | A |
| ATOM | 470 | CE1 | PHE | A | 58  | 39.992 | -8.792  | 26.765 | 1.00 | 21.25 | A |
| ATOM | 471 | CE2 | PHE | A | 58  | 41.393 | -7.207  | 25.610 | 1.00 | 20.28 | A |
| ATOM | 472 | CZ  | PHE | A | 58  | 40.457 | -8.238  | 25.578 | 1.00 | 21.18 | A |
| ATOM | 473 | C   | PHE | A | 58  | 44.278 | -7.401  | 28.612 | 1.00 | 21.79 | A |
| ATOM | 474 | O   | PHE | A | 58  | 44.529 | -8.260  | 27.763 | 1.00 | 21.84 | A |
| ATOM | 475 | N   | ALA | A | 59  | 44.849 | -6.202  | 28.637 | 1.00 | 21.80 | A |
| ATOM | 476 | CA  | ALA | A | 59  | 45.840 | -5.801  | 27.657 | 1.00 | 21.67 | A |
| ATOM | 477 | CB  | ALA | A | 59  | 46.254 | -4.346  | 27.892 | 1.00 | 21.11 | A |
| ATOM | 478 | C   | ALA | A | 59  | 47.053 | -6.711  | 27.732 | 1.00 | 22.06 | A |
| ATOM | 479 | O   | ALA | A | 59  | 47.518 | -7.213  | 26.706 | 1.00 | 22.53 | A |
| ATOM | 480 | N   | LEU | A | 60  | 47.561 | -6.925  | 28.945 | 1.00 | 19.83 | A |
| ATOM | 481 | CA  | LEU | A | 60  | 48.729 | -7.777  | 29.116 | 1.00 | 20.88 | A |
| ATOM | 482 | CB  | LEU | A | 60  | 49.163 | -7.815  | 30.585 | 1.00 | 20.57 | A |
| ATOM | 483 | CG  | LEU | A | 60  | 50.060 | -6.657  | 31.053 | 1.00 | 24.17 | A |
| ATOM | 484 | CD1 | LEU | A | 60  | 49.239 | -5.392  | 31.205 | 1.00 | 24.16 | A |
| ATOM | 485 | CD2 | LEU | A | 60  | 50.717 | -7.012  | 32.382 | 1.00 | 24.31 | A |
| ATOM | 486 | C   | LEU | A | 60  | 48.496 | -9.193  | 28.598 | 1.00 | 20.44 | A |
| ATOM | 487 | O   | LEU | A | 60  | 49.367 | -9.770  | 27.955 | 1.00 | 21.97 | A |
| ATOM | 488 | N   | THR | A | 61  | 47.319 | -9.749  | 28.871 | 1.00 | 20.69 | A |
| ATOM | 489 | CA  | THR | A | 61  | 46.997 | -11.101 | 28.418 | 1.00 | 19.49 | A |
| ATOM | 490 | CB  | THR | A | 61  | 45.697 | -11.629 | 29.084 | 1.00 | 18.59 | A |
| ATOM | 491 | OG1 | THR | A | 61  | 45.919 | -11.830 | 30.489 | 1.00 | 21.12 | A |
| ATOM | 492 | CG2 | THR | A | 61  | 45.274 | -12.942 | 28.453 | 1.00 | 17.61 | A |
| ATOM | 493 | C   | THR | A | 61  | 46.834 | -11.140 | 26.903 | 1.00 | 19.22 | A |
| ATOM | 494 | O   | THR | A | 61  | 47.325 | -12.059 | 26.242 | 1.00 | 21.19 | A |
| ATOM | 495 | N   | ASN | A | 62  | 46.152 | -10.142 | 26.351 | 1.00 | 18.05 | A |
| ATOM | 496 | CA  | ASN | A | 62  | 45.934 | -10.092 | 24.910 | 1.00 | 19.26 | A |
| ATOM | 497 | CB  | ASN | A | 62  | 45.020 | -8.910  | 24.552 | 1.00 | 20.51 | A |
| ATOM | 498 | CG  | ASN | A | 62  | 43.835 | -9.324  | 23.680 | 1.00 | 22.06 | A |
| ATOM | 499 | OD1 | ASN | A | 62  | 43.406 | -10.482 | 23.693 | 1.00 | 21.71 | A |
| ATOM | 500 | ND2 | ASN | A | 62  | 43.294 | -8.371  | 22.930 | 1.00 | 20.64 | A |
| ATOM | 501 | C   | ASN | A | 62  | 47.270 | -9.975  | 24.188 | 1.00 | 18.14 | A |
| ATOM | 502 | O   | ASN | A | 62  | 47.517 | -10.681 | 23.217 | 1.00 | 19.73 | A |
| ATOM | 503 | N   | ILE | A | 63  | 48.146 | -9.108  | 24.684 | 1.00 | 18.98 | A |
| ATOM | 504 | CA  | ILE | A | 63  | 49.448 | -8.921  | 24.061 | 1.00 | 19.88 | A |
| ATOM | 505 | CB  | ILE | A | 63  | 50.229 | -7.757  | 24.725 | 1.00 | 21.31 | A |
| ATOM | 506 | CG2 | ILE | A | 63  | 51.601 | -7.590  | 24.064 | 1.00 | 20.11 | A |
| ATOM | 507 | CG1 | ILE | A | 63  | 49.425 | -6.457  | 24.599 | 1.00 | 20.91 | A |
| ATOM | 508 | CD1 | ILE | A | 63  | 49.037 | -6.092  | 23.171 | 1.00 | 16.67 | A |
| ATOM | 509 | C   | ILE | A | 63  | 50.247 | -10.212 | 24.169 | 1.00 | 20.35 | A |
| ATOM | 510 | O   | ILE | A | 63  | 51.048 | -10.538 | 23.297 | 1.00 | 21.37 | A |
| ATOM | 511 | N   | ALA | A | 64  | 50.028 | -10.949 | 25.247 | 1.00 | 22.48 | A |
| ATOM | 512 | CA  | ALA | A | 64  | 50.713 | -12.222 | 25.423 | 1.00 | 23.35 | A |
| ATOM | 513 | CB  | ALA | A | 64  | 50.373 | -12.816 | 26.785 | 1.00 | 22.29 | A |

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ATOM    514  C   ALA A  64      50.252 -13.158  24.301  1.00 23.03           A
ATOM    515  O   ALA A  64      51.032 -13.939  23.766  1.00 25.08           A
ATOM    516  N   VAL A  65      48.976 -13.072  23.948  1.00 23.28           A
ATOM    517  CA  VAL A  65      48.437 -13.905  22.888  1.00 22.97           A
ATOM    518  CB  VAL A  65      46.887 -13.840  22.859  1.00 24.28           A
ATOM    519  CG1 VAL A  65      46.338 -14.722  21.729  1.00 22.40           A
ATOM    520  CG2 VAL A  65      46.325 -14.296  24.209  1.00 19.61           A
ATOM    521  C   VAL A  65      49.013 -13.471  21.538  1.00 23.88           A
ATOM    522  O   VAL A  65      49.313 -14.314  20.692  1.00 22.01           A
ATOM    523  N   LEU A  66      49.179 -12.164  21.332  1.00 24.00           A
ATOM    524  CA  LEU A  66      49.747 -11.692  20.064  1.00 24.66           A
ATOM    525  CB  LEU A  66      49.872 -10.171  20.011  1.00 22.13           A
ATOM    526  CG  LEU A  66      48.679  -9.228  20.117  1.00 23.81           A
ATOM    527  CD1 LEU A  66      49.014  -8.001  19.277  1.00 20.24           A
ATOM    528  CD2 LEU A  66      47.407  -9.866  19.627  1.00 20.49           A
ATOM    529  C   LEU A  66      51.143 -12.267  19.906  1.00 23.53           A
ATOM    530  O   LEU A  66      51.548 -12.644  18.813  1.00 22.08           A
ATOM    531  N   LYS A  67      51.879 -12.303  21.011  1.00 26.17           A
ATOM    532  CA  LYS A  67      53.237 -12.832  21.019  1.00 28.99           A
ATOM    533  CB  LYS A  67      53.839 -12.698  22.421  1.00 29.27           A
ATOM    534  CG  LYS A  67      55.278 -13.174  22.548  1.00 30.64           A
ATOM    535  CD  LYS A  67      55.779 -13.001  23.976  1.00 32.41           A
ATOM    536  CE  LYS A  67      57.159 -13.609  24.157  1.00 35.25           A
ATOM    537  NZ  LYS A  67      58.144 -13.036  23.199  1.00 38.78           A
ATOM    538  C   LYS A  67      53.200 -14.299  20.598  1.00 29.87           A
ATOM    539  O   LYS A  67      53.952 -14.719  19.716  1.00 30.35           A
ATOM    540  N   HIS A  68      52.313 -15.066  21.230  1.00 30.48           A
ATOM    541  CA  HIS A  68      52.163 -16.483  20.922  1.00 31.95           A
ATOM    542  CB  HIS A  68      51.051 -17.097  21.775  1.00 34.42           A
ATOM    543  CG  HIS A  68      50.827 -18.557  21.520  1.00 38.63           A
ATOM    544  CD2 HIS A  68      49.859 -19.203  20.826  1.00 40.18           A
ATOM    545  ND1 HIS A  68      51.676 -19.536  21.992  1.00 41.00           A
ATOM    546  CE1 HIS A  68      51.241 -20.721  21.601  1.00 39.93           A
ATOM    547  NE2 HIS A  68      50.141 -20.547  20.891  1.00 39.69           A
ATOM    548  C   HIS A  68      51.828 -16.660  19.448  1.00 31.53           A
ATOM    549  O   HIS A  68      52.463 -17.447  18.746  1.00 32.07           A
ATOM    550  N   ASN A  69      50.826 -15.928  18.977  1.00 29.53           A
ATOM    551  CA  ASN A  69      50.427 -16.024  17.583  1.00 29.99           A
ATOM    552  CB  ASN A  69      49.180 -15.173  17.332  1.00 30.27           A
ATOM    553  CG  ASN A  69      47.918 -15.814  17.885  1.00 31.83           A
ATOM    554  OD1 ASN A  69      47.986 -16.728  18.703  1.00 32.19           A
ATOM    555  ND2 ASN A  69      46.759 -15.328  17.447  1.00 31.41           A
ATOM    556  C   ASN A  69      51.552 -15.602  16.638  1.00 30.37           A
ATOM    557  O   ASN A  69      51.722 -16.186  15.571  1.00 29.41           A
ATOM    558  N   LEU A  70      52.324 -14.593  17.026  1.00 29.86           A
ATOM    559  CA  LEU A  70      53.413 -14.131  16.175  1.00 31.35           A
ATOM    560  CB  LEU A  70      54.039 -12.857  16.751  1.00 28.55           A
ATOM    561  CG  LEU A  70      55.190 -12.237  15.950  1.00 28.77           A
ATOM    562  CD1 LEU A  70      54.745 -11.949  14.519  1.00 28.48           A
ATOM    563  CD2 LEU A  70      55.651 -10.957  16.627  1.00 27.89           A
ATOM    564  C   LEU A  70      54.479 -15.214  16.009  1.00 31.92           A
ATOM    565  O   LEU A  70      54.994 -15.422  14.914  1.00 31.72           A
ATOM    566  N   ASN A  71      54.798 -15.905  17.097  1.00 34.09           A
ATOM    567  CA  ASN A  71      55.801 -16.968  17.060  1.00 38.27           A
ATOM    568  CB  ASN A  71      55.884 -17.651  18.427  1.00 39.70           A
ATOM    569  CG  ASN A  71      56.490 -16.748  19.490  1.00 44.05           A
ATOM    570  OD1 ASN A  71      56.290 -16.955  20.693  1.00 44.98           A
ATOM    571  ND2 ASN A  71      57.247 -15.746  19.049  1.00 44.44           A
ATOM    572  C   ASN A  71      55.484 -18.003  15.983  1.00 38.32           A
ATOM    573  O   ASN A  71      56.358 -18.417  15.224  1.00 37.91           A
ATOM    574  N   SER A  72      54.221 -18.407  15.919  1.00 39.49           A
ATOM    575  CA  SER A  72      53.780 -19.390  14.944  1.00 40.10           A
ATOM    576  CB  SER A  72      52.341 -19.816  15.256  1.00 41.05           A
ATOM    577  OG  SER A  72      51.867 -20.763  14.311  1.00 42.44           A
ATOM    578  C   SER A  72      53.860 -18.838  13.523  1.00 40.66           A
ATOM    579  O   SER A  72      54.336 -19.516  12.608  1.00 40.90           A
ATOM    580  N   LEU A  73      53.391 -17.608  13.341  1.00 39.86           A
ATOM    581  CA  LEU A  73      53.408 -16.973  12.030  1.00 39.32           A
ATOM    582  CB  LEU A  73      52.676 -15.632  12.082  1.00 38.99           A
ATOM    583  CG  LEU A  73      51.221 -15.651  11.598  1.00 40.31           A
ATOM    584  CD1 LEU A  73      50.482 -16.860  12.152  1.00 39.79           A
ATOM    585  CD2 LEU A  73      50.539 -14.363  12.024  1.00 40.04           A
ATOM    586  C   LEU A  73      54.816 -16.778  11.492  1.00 38.55           A
ATOM    587  O   LEU A  73      55.028 -16.806  10.280  1.00 36.83           A
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| ATOM | 588 | N | ILE A | 74 | 55.780 | -16.576 | 12.383 | 1.00 | 39.70 | A |
| ATOM | 589 | CA | ILE A | 74 | 57.158 | -16.402 | 11.942 | 1.00 | 41.87 | A |
| ATOM | 590 | CB | ILE A | 74 | 58.104 | -16.084 | 13.123 | 1.00 | 41.88 | A |
| ATOM | 591 | CG2 | ILE A | 74 | 59.552 | -16.054 | 12.640 | 1.00 | 41.29 | A |
| ATOM | 592 | CG1 | ILE A | 74 | 57.729 | -14.734 | 13.738 | 1.00 | 41.53 | A |
| ATOM | 593 | CD1 | ILE A | 74 | 58.519 | -14.380 | 14.990 | 1.00 | 40.94 | A |
| ATOM | 594 | C | ILE A | 74 | 57.599 | -17.699 | 11.273 | 1.00 | 42.04 | A |
| ATOM | 595 | O | ILE A | 74 | 58.119 | -17.689 | 10.157 | 1.00 | 41.12 | A |
| ATOM | 596 | N | LYS A | 75 | 57.364 | -18.816 | 11.954 | 1.00 | 43.51 | A |
| ATOM | 597 | CA | LYS A | 75 | 57.730 | -20.125 | 11.423 | 1.00 | 46.61 | A |
| ATOM | 598 | CB | LYS A | 75 | 57.470 | -21.217 | 12.466 | 1.00 | 47.84 | A |
| ATOM | 599 | CG | LYS A | 75 | 58.096 | -20.964 | 13.828 | 1.00 | 50.82 | A |
| ATOM | 600 | CD | LYS A | 75 | 57.661 | -22.029 | 14.828 | 1.00 | 53.97 | A |
| ATOM | 601 | CE | LYS A | 75 | 58.005 | -21.646 | 16.269 | 1.00 | 55.95 | A |
| ATOM | 602 | NZ | LYS A | 75 | 59.472 | -21.572 | 16.531 | 1.00 | 56.31 | A |
| ATOM | 603 | C | LYS A | 75 | 56.944 | -20.452 | 10.151 | 1.00 | 47.99 | A |
| ATOM | 604 | O | LYS A | 75 | 57.530 | -20.720 | 9.106 | 1.00 | 48.11 | A |
| ATOM | 605 | N | ARG A | 76 | 55.617 | -20.419 | 10.242 | 1.00 | 49.31 | A |
| ATOM | 606 | CA | ARG A | 76 | 54.763 | -20.742 | 9.103 | 1.00 | 50.89 | A |
| ATOM | 607 | CB | ARG A | 76 | 53.287 | -20.744 | 9.530 | 1.00 | 53.08 | A |
| ATOM | 608 | CG | ARG A | 76 | 52.960 | -21.847 | 10.538 | 1.00 | 56.83 | A |
| ATOM | 609 | CD | ARG A | 76 | 51.478 | -22.247 | 10.574 | 1.00 | 58.85 | A |
| ATOM | 610 | NE | ARG A | 76 | 50.620 | -21.253 | 11.212 | 1.00 | 60.24 | A |
| ATOM | 611 | CZ | ARG A | 76 | 49.786 | -20.452 | 10.557 | 1.00 | 61.29 | A |
| ATOM | 612 | NH1 | ARG A | 76 | 49.692 | -20.526 | 9.234 | 1.00 | 60.08 | A |
| ATOM | 613 | NH2 | ARG A | 76 | 49.044 | -19.578 | 11.226 | 1.00 | 61.97 | A |
| ATOM | 614 | C | ARG A | 76 | 54.947 | -19.871 | 7.864 | 1.00 | 50.93 | A |
| ATOM | 615 | O | ARG A | 76 | 54.705 | -20.324 | 6.747 | 1.00 | 51.19 | A |
| ATOM | 616 | N | SER A | 77 | 55.380 | -18.630 | 8.046 | 1.00 | 50.61 | A |
| ATOM | 617 | CA | SER A | 77 | 55.574 | -17.745 | 6.900 | 1.00 | 50.08 | A |
| ATOM | 618 | CB | SER A | 77 | 55.262 | -16.295 | 7.282 | 1.00 | 50.05 | A |
| ATOM | 619 | OG | SER A | 77 | 56.223 | -15.787 | 8.193 | 1.00 | 49.23 | A |
| ATOM | 620 | C | SER A | 77 | 57.006 | -17.827 | 6.386 | 1.00 | 49.56 | A |
| ATOM | 621 | O | SER A | 77 | 57.420 | -17.015 | 5.558 | 1.00 | 49.40 | A |
| ATOM | 622 | N | ASN A | 78 | 57.752 | -18.817 | 6.866 | 1.00 | 49.24 | A |
| ATOM | 623 | CA | ASN A | 78 | 59.148 | -18.982 | 6.472 | 1.00 | 49.14 | A |
| ATOM | 624 | CB | ASN A | 78 | 59.256 | -19.307 | 4.976 | 1.00 | 48.86 | A |
| ATOM | 625 | CG | ASN A | 78 | 60.668 | -19.689 | 4.558 | 1.00 | 48.09 | A |
| ATOM | 626 | OD1 | ASN A | 78 | 61.347 | -20.442 | 5.254 | 1.00 | 46.05 | A |
| ATOM | 627 | ND2 | ASN A | 78 | 61.109 | -19.182 | 3.409 | 1.00 | 47.78 | A |
| ATOM | 628 | C | ASN A | 78 | 59.857 | -17.667 | 6.803 | 1.00 | 49.08 | A |
| ATOM | 629 | O | ASN A | 78 | 60.614 | -17.114 | 6.001 | 1.00 | 48.39 | A |
| ATOM | 630 | N | SER A | 79 | 59.571 | -17.177 | 8.006 | 1.00 | 48.58 | A |
| ATOM | 631 | CA | SER A | 79 | 60.139 | -15.945 | 8.538 | 1.00 | 48.38 | A |
| ATOM | 632 | CB | SER A | 79 | 61.549 | -16.208 | 9.071 | 1.00 | 48.53 | A |
| ATOM | 633 | OG | SER A | 79 | 62.415 | -16.612 | 8.027 | 1.00 | 50.05 | A |
| ATOM | 634 | C | SER A | 79 | 60.176 | -14.768 | 7.573 | 1.00 | 47.13 | A |
| ATOM | 635 | O | SER A | 79 | 61.197 | -14.098 | 7.444 | 1.00 | 47.66 | A |
| ATOM | 636 | N | THR A | 80 | 59.069 | -14.516 | 6.887 | 1.00 | 45.82 | A |
| ATOM | 637 | CA | THR A | 80 | 59.008 | -13.379 | 5.982 | 1.00 | 45.51 | A |
| ATOM | 638 | CB | THR A | 80 | 57.814 | -13.501 | 5.016 | 1.00 | 47.03 | A |
| ATOM | 639 | OG1 | THR A | 80 | 56.663 | -13.963 | 5.731 | 1.00 | 47.95 | A |
| ATOM | 640 | CG2 | THR A | 80 | 58.134 | -14.487 | 3.909 | 1.00 | 47.59 | A |
| ATOM | 641 | C | THR A | 80 | 58.855 | -12.147 | 6.882 | 1.00 | 44.25 | A |
| ATOM | 642 | O | THR A | 80 | 57.835 | -11.976 | 7.556 | 1.00 | 43.69 | A |
| ATOM | 643 | N | ALA A | 81 | 59.889 | -11.311 | 6.903 | 1.00 | 41.47 | A |
| ATOM | 644 | CA | ALA A | 81 | 59.916 | -10.119 | 7.740 | 1.00 | 38.59 | A |
| ATOM | 645 | CB | ALA A | 81 | 61.363 | -9.734 | 8.039 | 1.00 | 38.61 | A |
| ATOM | 646 | C | ALA A | 81 | 59.168 | -8.915 | 7.185 | 1.00 | 36.89 | A |
| ATOM | 647 | O | ALA A | 81 | 58.766 | -8.884 | 6.018 | 1.00 | 35.83 | A |
| ATOM | 648 | N | ALA A | 82 | 58.993 | -7.920 | 8.050 | 1.00 | 34.86 | A |
| ATOM | 649 | CA | ALA A | 82 | 58.300 | -6.690 | 7.698 | 1.00 | 33.41 | A |
| ATOM | 650 | CB | ALA A | 82 | 57.957 | -5.912 | 8.961 | 1.00 | 34.17 | A |
| ATOM | 651 | C | ALA A | 82 | 59.141 | -5.824 | 6.770 | 1.00 | 32.28 | A |
| ATOM | 652 | O | ALA A | 82 | 60.372 | -5.807 | 6.859 | 1.00 | 28.62 | A |
| ATOM | 653 | N | THR A | 83 | 58.457 | -5.113 | 5.878 | 1.00 | 31.60 | A |
| ATOM | 654 | CA | THR A | 83 | 59.100 | -4.217 | 4.931 | 1.00 | 32.87 | A |
| ATOM | 655 | CB | THR A | 83 | 58.377 | -4.224 | 3.575 | 1.00 | 34.31 | A |
| ATOM | 656 | OG1 | THR A | 83 | 58.347 | -5.562 | 3.058 | 1.00 | 36.90 | A |
| ATOM | 657 | CG2 | THR A | 83 | 59.098 | -3.309 | 2.578 | 1.00 | 34.35 | A |
| ATOM | 658 | C | THR A | 83 | 59.041 | -2.808 | 5.500 | 1.00 | 32.84 | A |
| ATOM | 659 | O | THR A | 83 | 58.029 | -2.406 | 6.067 | 1.00 | 33.97 | A |
| ATOM | 660 | N | ASN A | 84 | 60.130 | -2.062 | 5.356 | 1.00 | 34.76 | A |
| ATOM | 661 | CA | ASN A | 84 | 60.188 | -0.697 | 5.858 | 1.00 | 34.66 | A |

| ATOM | 662 | CB | ASN A | 84 | 61.634 | -0.252 | 6.069 | 1.00 | 36.13 | A |
|------|-----|-----|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 663 | CG | ASN A | 84 | 62.337 | -1.045 | 7.132 | 1.00 | 37.22 | A |
| ATOM | 664 | OD1 | ASN A | 84 | 61.809 | -1.241 | 8.220 | 1.00 | 39.34 | A |
| ATOM | 665 | ND2 | ASN A | 84 | 63.548 | -1.497 | 6.830 | 1.00 | 38.89 | A |
| ATOM | 666 | C | ASN A | 84 | 59.549 | 0.267 | 4.881 | 1.00 | 35.51 | A |
| ATOM | 667 | O | ASN A | 84 | 59.961 | 0.343 | 3.724 | 1.00 | 38.89 | A |
| ATOM | 668 | N | GLU A | 85 | 58.546 | 1.004 | 5.344 | 1.00 | 34.17 | A |
| ATOM | 669 | CA | GLU A | 85 | 57.890 | 2.001 | 4.507 | 1.00 | 32.82 | A |
| ATOM | 670 | CB | GLU A | 85 | 56.427 | 2.183 | 4.921 | 1.00 | 36.55 | A |
| ATOM | 671 | CG | GLU A | 85 | 55.523 | 0.993 | 4.645 | 1.00 | 42.74 | A |
| ATOM | 672 | CD | GLU A | 85 | 55.271 | 0.782 | 3.167 | 1.00 | 46.65 | A |
| ATOM | 673 | OE1 | GLU A | 85 | 54.829 | 1.741 | 2.494 | 1.00 | 49.22 | A |
| ATOM | 674 | OE2 | GLU A | 85 | 55.508 | -0.345 | 2.679 | 1.00 | 48.74 | A |
| ATOM | 675 | C | GLU A | 85 | 58.624 | 3.328 | 4.701 | 1.00 | 30.10 | A |
| ATOM | 676 | O | GLU A | 85 | 59.489 | 3.453 | 5.571 | 1.00 | 27.29 | A |
| ATOM | 677 | N | VAL A | 86 | 58.274 | 4.308 | 3.878 | 1.00 | 28.67 | A |
| ATOM | 678 | CA | VAL A | 86 | 58.849 | 5.641 | 3.951 | 1.00 | 27.33 | A |
| ATOM | 679 | CB | VAL A | 86 | 59.146 | 6.202 | 2.539 | 1.00 | 27.74 | A |
| ATOM | 680 | CG1 | VAL A | 86 | 59.688 | 7.637 | 2.640 | 1.00 | 22.06 | A |
| ATOM | 681 | CG2 | VAL A | 86 | 60.139 | 5.289 | 1.815 | 1.00 | 25.30 | A |
| ATOM | 682 | C | VAL A | 86 | 57.786 | 6.519 | 4.614 | 1.00 | 27.98 | A |
| ATOM | 683 | O | VAL A | 86 | 56.685 | 6.671 | 4.086 | 1.00 | 28.76 | A |
| ATOM | 684 | N | PRO A | 87 | 58.095 | 7.098 | 5.784 | 1.00 | 27.39 | A |
| ATOM | 685 | CD | PRO A | 87 | 59.268 | 6.861 | 6.644 | 1.00 | 26.00 | A |
| ATOM | 686 | CA | PRO A | 87 | 57.106 | 7.949 | 6.458 | 1.00 | 28.38 | A |
| ATOM | 687 | CB | PRO A | 87 | 57.611 | 7.989 | 7.899 | 1.00 | 26.97 | A |
| ATOM | 688 | CG | PRO A | 87 | 59.099 | 7.915 | 7.727 | 1.00 | 27.97 | A |
| ATOM | 689 | C | PRO A | 87 | 56.963 | 9.341 | 5.848 | 1.00 | 30.15 | A |
| ATOM | 690 | O | PRO A | 87 | 57.902 | 9.871 | 5.245 | 1.00 | 31.62 | A |
| ATOM | 691 | N | GLU A | 88 | 55.778 | 9.922 | 6.004 | 1.00 | 29.70 | A |
| ATOM | 692 | CA | GLU A | 88 | 55.489 | 11.252 | 5.481 | 1.00 | 29.65 | A |
| ATOM | 693 | CB | GLU A | 88 | 54.173 | 11.229 | 4.699 | 1.00 | 32.09 | A |
| ATOM | 694 | CG | GLU A | 88 | 54.038 | 12.330 | 3.655 | 1.00 | 38.40 | A |
| ATOM | 695 | CD | GLU A | 88 | 52.790 | 12.172 | 2.792 | 1.00 | 41.07 | A |
| ATOM | 696 | OE1 | GLU A | 88 | 51.675 | 12.411 | 3.303 | 1.00 | 42.35 | A |
| ATOM | 697 | OE2 | GLU A | 88 | 52.925 | 11.800 | 1.604 | 1.00 | 43.46 | A |
| ATOM | 698 | C | GLU A | 88 | 55.385 | 12.191 | 6.680 | 1.00 | 27.98 | A |
| ATOM | 699 | O | GLU A | 88 | 54.588 | 11.954 | 7.597 | 1.00 | 26.16 | A |
| ATOM | 700 | N | VAL A | 89 | 56.187 | 13.253 | 6.672 | 1.00 | 23.90 | A |
| ATOM | 701 | CA | VAL A | 89 | 56.201 | 14.194 | 7.788 | 1.00 | 21.62 | A |
| ATOM | 702 | CB | VAL A | 89 | 57.637 | 14.358 | 8.333 | 1.00 | 18.36 | A |
| ATOM | 703 | CG1 | VAL A | 89 | 57.639 | 15.295 | 9.534 | 1.00 | 17.11 | A |
| ATOM | 704 | CG2 | VAL A | 89 | 58.204 | 12.990 | 8.719 | 1.00 | 16.77 | A |
| ATOM | 705 | C | VAL A | 89 | 55.626 | 15.575 | 7.483 | 1.00 | 21.60 | A |
| ATOM | 706 | O | VAL A | 89 | 55.859 | 16.143 | 6.420 | 1.00 | 21.72 | A |
| ATOM | 707 | N | THR A | 90 | 54.886 | 16.115 | 8.444 | 1.00 | 21.28 | A |
| ATOM | 708 | CA | THR A | 90 | 54.269 | 17.425 | 8.301 | 1.00 | 20.62 | A |
| ATOM | 709 | CB | THR A | 90 | 52.813 | 17.303 | 7.823 | 1.00 | 21.90 | A |
| ATOM | 710 | OG1 | THR A | 90 | 52.770 | 16.537 | 6.613 | 1.00 | 26.43 | A |
| ATOM | 711 | CG2 | THR A | 90 | 52.220 | 18.678 | 7.558 | 1.00 | 23.70 | A |
| ATOM | 712 | C | THR A | 90 | 54.264 | 18.153 | 9.639 | 1.00 | 21.08 | A |
| ATOM | 713 | O | THR A | 90 | 53.887 | 17.578 | 10.667 | 1.00 | 20.41 | A |
| ATOM | 714 | N | VAL A | 91 | 54.670 | 19.423 | 9.618 | 1.00 | 19.24 | A |
| ATOM | 715 | CA | VAL A | 91 | 54.712 | 20.243 | 10.822 | 1.00 | 19.55 | A |
| ATOM | 716 | CB | VAL A | 91 | 56.149 | 20.739 | 11.102 | 1.00 | 19.97 | A |
| ATOM | 717 | CG1 | VAL A | 91 | 56.167 | 21.629 | 12.338 | 1.00 | 16.82 | A |
| ATOM | 718 | CG2 | VAL A | 91 | 57.072 | 19.547 | 11.280 | 1.00 | 17.43 | A |
| ATOM | 719 | C | VAL A | 91 | 53.789 | 21.452 | 10.703 | 1.00 | 19.10 | A |
| ATOM | 720 | O | VAL A | 91 | 53.735 | 22.108 | 9.666 | 1.00 | 20.59 | A |
| ATOM | 721 | N | PHE A | 92 | 53.059 | 21.739 | 11.772 | 1.00 | 18.65 | A |
| ATOM | 722 | CA | PHE A | 92 | 52.146 | 22.870 | 11.785 | 1.00 | 19.10 | A |
| ATOM | 723 | CB | PHE A | 92 | 50.853 | 22.516 | 11.030 | 1.00 | 18.89 | A |
| ATOM | 724 | CG | PHE A | 92 | 50.176 | 21.264 | 11.525 | 1.00 | 16.16 | A |
| ATOM | 725 | CD1 | PHE A | 92 | 49.165 | 21.331 | 12.480 | 1.00 | 16.77 | A |
| ATOM | 726 | CD2 | PHE A | 92 | 50.561 | 20.017 | 11.047 | 1.00 | 16.62 | A |
| ATOM | 727 | CE1 | PHE A | 92 | 48.543 | 20.168 | 12.955 | 1.00 | 18.06 | A |
| ATOM | 728 | CE2 | PHE A | 92 | 49.954 | 18.848 | 11.511 | 1.00 | 18.17 | A |
| ATOM | 729 | CZ | PHE A | 92 | 48.936 | 18.922 | 12.471 | 1.00 | 17.05 | A |
| ATOM | 730 | C | PHE A | 92 | 51.844 | 23.236 | 13.229 | 1.00 | 19.48 | A |
| ATOM | 731 | O | PHE A | 92 | 52.055 | 22.430 | 14.134 | 1.00 | 19.64 | A |
| ATOM | 732 | N | SER A | 93 | 51.365 | 24.453 | 13.445 | 1.00 | 18.69 | A |
| ATOM | 733 | CA | SER A | 93 | 51.052 | 24.896 | 14.792 | 1.00 | 19.26 | A |
| ATOM | 734 | CB | SER A | 93 | 51.275 | 26.408 | 14.921 | 1.00 | 17.24 | A |
| ATOM | 735 | OG | SER A | 93 | 50.435 | 27.132 | 14.043 | 1.00 | 20.17 | A |

| ATOM | 736 | C | SER A | 93 | 49.618 | 24.554 | 15.172 | 1.00 | 19.04 | A |
|------|-----|------|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 737 | O | SER A | 93 | 48.748 | 24.417 | 14.316 | 1.00 | 17.44 | A |
| ATOM | 738 | N | LYS A | 94 | 49.390 | 24.418 | 16.472 | 1.00 | 20.26 | A |
| ATOM | 739 | CA | LYS A | 94 | 48.077 | 24.108 | 17.010 | 1.00 | 21.70 | A |
| ATOM | 740 | CB | LYS A | 94 | 48.227 | 23.670 | 18.464 | 1.00 | 22.45 | A |
| ATOM | 741 | CG | LYS A | 94 | 46.938 | 23.273 | 19.139 | 1.00 | 24.42 | A |
| ATOM | 742 | CD | LYS A | 94 | 47.189 | 22.867 | 20.587 | 1.00 | 25.48 | A |
| ATOM | 743 | CE | LYS A | 94 | 45.881 | 22.548 | 21.297 | 1.00 | 25.73 | A |
| ATOM | 744 | NZ | LYS A | 94 | 45.122 | 21.533 | 20.517 | 1.00 | 26.34 | A |
| ATOM | 745 | C | LYS A | 94 | 47.169 | 25.340 | 16.921 | 1.00 | 23.44 | A |
| ATOM | 746 | O | LYS A | 94 | 45.984 | 25.235 | 16.598 | 1.00 | 20.95 | A |
| ATOM | 747 | N | SER A | 95 | 47.742 | 26.505 | 17.212 | 1.00 | 24.82 | A |
| ATOM | 748 | CA | SER A | 95 | 47.013 | 27.769 | 17.172 | 1.00 | 27.69 | A |
| ATOM | 749 | CB | SER A | 95 | 46.969 | 28.408 | 18.565 | 1.00 | 26.33 | A |
| ATOM | 750 | OG | SER A | 95 | 46.202 | 27.635 | 19.468 | 1.00 | 32.56 | A |
| ATOM | 751 | C | SER A | 95 | 47.688 | 28.747 | 16.219 | 1.00 | 27.36 | A |
| ATOM | 752 | O | SER A | 95 | 48.824 | 28.529 | 15.797 | 1.00 | 27.94 | A |
| ATOM | 753 | N | PRO A | 96 | 46.985 | 29.830 | 15.849 | 1.00 | 27.27 | A |
| ATOM | 754 | CD | PRO A | 96 | 45.611 | 30.232 | 16.193 | 1.00 | 28.85 | A |
| ATOM | 755 | CA | PRO A | 96 | 47.606 | 30.801 | 14.946 | 1.00 | 26.90 | A |
| ATOM | 756 | CB | PRO A | 96 | 46.471 | 31.788 | 14.663 | 1.00 | 28.13 | A |
| ATOM | 757 | CG | PRO A | 96 | 45.634 | 31.719 | 15.907 | 1.00 | 28.36 | A |
| ATOM | 758 | C | PRO A | 96 | 48.786 | 31.421 | 15.700 | 1.00 | 24.92 | A |
| ATOM | 759 | O | PRO A | 96 | 48.757 | 31.556 | 16.925 | 1.00 | 24.65 | A |
| ATOM | 760 | N | VAL A | 97 | 49.828 | 31.786 | 14.973 | 1.00 | 24.24 | A |
| ATOM | 761 | CA | VAL A | 97 | 51.016 | 32.332 | 15.601 | 1.00 | 25.15 | A |
| ATOM | 762 | CB | VAL A | 97 | 52.261 | 32.087 | 14.715 | 1.00 | 26.78 | A |
| ATOM | 763 | CG1 | VAL A | 97 | 53.531 | 32.372 | 15.508 | 1.00 | 26.15 | A |
| ATOM | 764 | CG2 | VAL A | 97 | 52.255 | 30.659 | 14.198 | 1.00 | 26.15 | A |
| ATOM | 765 | C | VAL A | 97 | 50.935 | 33.820 | 15.920 | 1.00 | 25.62 | A |
| ATOM | 766 | O | VAL A | 97 | 50.624 | 34.638 | 15.054 | 1.00 | 25.01 | A |
| ATOM | 767 | N | THR A | 98 | 51.207 | 34.157 | 17.175 | 1.00 | 24.46 | A |
| ATOM | 768 | CA | THR A | 98 | 51.212 | 35.542 | 17.627 | 1.00 | 25.36 | A |
| ATOM | 769 | CB | THR A | 98 | 49.835 | 35.941 | 18.283 | 1.00 | 25.29 | A |
| ATOM | 770 | OG1 | THR A | 98 | 50.030 | 37.008 | 19.217 | 1.00 | 30.50 | A |
| ATOM | 771 | CG2 | THR A | 98 | 49.196 | 34.771 | 18.985 | 1.00 | 29.80 | A |
| ATOM | 772 | C | THR A | 98 | 52.382 | 35.678 | 18.605 | 1.00 | 24.87 | A |
| ATOM | 773 | O | THR A | 98 | 52.499 | 34.902 | 19.554 | 1.00 | 23.01 | A |
| ATOM | 774 | N | LEU A | 99 | 53.273 | 36.634 | 18.344 | 1.00 | 25.94 | A |
| ATOM | 775 | CA | LEU A | 99 | 54.445 | 36.843 | 19.198 | 1.00 | 28.02 | A |
| ATOM | 776 | CB | LEU A | 99 | 55.194 | 38.114 | 18.797 | 1.00 | 31.12 | A |
| ATOM | 777 | CG | LEU A | 99 | 55.950 | 38.211 | 17.469 | 1.00 | 35.44 | A |
| ATOM | 778 | CD1 | LEU A | 99 | 56.650 | 39.577 | 17.416 | 1.00 | 35.45 | A |
| ATOM | 779 | CD2 | LEU A | 99 | 56.970 | 37.087 | 17.341 | 1.00 | 35.62 | A |
| ATOM | 780 | C | LEU A | 99 | 54.135 | 36.932 | 20.689 | 1.00 | 27.10 | A |
| ATOM | 781 | O | LEU A | 99 | 53.201 | 37.616 | 21.097 | 1.00 | 25.34 | A |
| ATOM | 782 | N | GLY A | 100 | 54.935 | 36.233 | 21.492 | 1.00 | 26.71 | A |
| ATOM | 783 | CA | GLY A | 100 | 54.762 | 36.253 | 22.935 | 1.00 | 26.48 | A |
| ATOM | 784 | C | GLY A | 100 | 53.635 | 35.398 | 23.479 | 1.00 | 26.32 | A |
| ATOM | 785 | O | GLY A | 100 | 53.428 | 35.323 | 24.695 | 1.00 | 25.37 | A |
| ATOM | 786 | N | GLN A | 101 | 52.913 | 34.734 | 22.585 | 1.00 | 25.16 | A |
| ATOM | 787 | CA | GLN A | 101 | 51.796 | 33.896 | 22.999 | 1.00 | 25.74 | A |
| ATOM | 788 | CB | GLN A | 101 | 50.573 | 34.219 | 22.143 | 1.00 | 28.06 | A |
| ATOM | 789 | CG | GLN A | 101 | 49.258 | 33.911 | 22.814 | 1.00 | 30.50 | A |
| ATOM | 790 | CD | GLN A | 101 | 49.123 | 34.599 | 24.162 | 1.00 | 32.88 | A |
| ATOM | 791 | OE1 | GLN A | 101 | 48.953 | 35.820 | 24.251 | 1.00 | 30.83 | A |
| ATOM | 792 | NE2 | GLN A | 101 | 49.202 | 33.813 | 25.221 | 1.00 | 33.04 | A |
| ATOM | 793 | C | GLN A | 101 | 52.117 | 32.409 | 22.901 | 1.00 | 24.01 | A |
| ATOM | 794 | O | GLN A | 101 | 52.280 | 31.881 | 21.807 | 1.00 | 24.25 | A |
| ATOM | 795 | N | PRO A | 102 | 52.199 | 31.715 | 24.051 | 1.00 | 22.08 | A |
| ATOM | 796 | CD | PRO A | 102 | 51.959 | 32.244 | 25.410 | 1.00 | 22.41 | A |
| ATOM | 797 | CA | PRO A | 102 | 52.500 | 30.278 | 24.096 | 1.00 | 21.37 | A |
| ATOM | 798 | CB | PRO A | 102 | 52.136 | 29.898 | 25.526 | 1.00 | 21.61 | A |
| ATOM | 799 | CG | PRO A | 102 | 52.521 | 31.147 | 26.297 | 1.00 | 21.90 | A |
| ATOM | 800 | C | PRO A | 102 | 51.706 | 29.480 | 23.068 | 1.00 | 21.30 | A |
| ATOM | 801 | O | PRO A | 102 | 50.496 | 29.644 | 22.947 | 1.00 | 21.93 | A |
| ATOM | 802 | N | ASN A | 103 | 52.396 | 28.618 | 22.327 | 1.00 | 18.86 | A |
| ATOM | 803 | CA | ASN A | 103 | 51.749 | 27.802 | 21.305 | 1.00 | 17.69 | A |
| ATOM | 804 | CB | ASN A | 103 | 52.040 | 28.379 | 19.913 | 1.00 | 17.99 | A |
| ATOM | 805 | CG | ASN A | 103 | 50.899 | 28.162 | 18.929 | 1.00 | 18.28 | A |
| ATOM | 806 | OD1 | ASN A | 103 | 50.348 | 27.060 | 18.808 | 1.00 | 17.82 | A |
| ATOM | 807 | ND2 | ASN A | 103 | 50.549 | 29.223 | 18.204 | 1.00 | 17.71 | A |
| ATOM | 808 | C | ASN A | 103 | 52.281 | 26.370 | 21.385 | 1.00 | 15.57 | A |
| ATOM | 809 | O | ASN A | 103 | 53.000 | 26.012 | 22.310 | 1.00 | 14.67 | A |

| ATOM | 810 | N | ILE A 104 | 51.918 | 25.565 | 20.397 | 1.00 | 15.80 | A |
|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 811 | CA | ILE A 104 | 52.335 | 24.177 | 20.328 | 1.00 | 13.66 | A |
| ATOM | 812 | CB | ILE A 104 | 51.255 | 23.235 | 20.888 | 1.00 | 15.40 | A |
| ATOM | 813 | CG2 | ILE A 104 | 51.589 | 21.792 | 20.539 | 1.00 | 13.82 | A |
| ATOM | 814 | CG1 | ILE A 104 | 51.132 | 23.421 | 22.400 | 1.00 | 17.40 | A |
| ATOM | 815 | CD1 | ILE A 104 | 50.129 | 22.494 | 23.047 | 1.00 | 18.65 | A |
| ATOM | 816 | C | ILE A 104 | 52.588 | 23.775 | 18.896 | 1.00 | 14.36 | A |
| ATOM | 817 | O | ILE A 104 | 51.716 | 23.924 | 18.052 | 1.00 | 16.86 | A |
| ATOM | 818 | N | LEU A 105 | 53.785 | 23.272 | 18.616 | 1.00 | 15.67 | A |
| ATOM | 819 | CA | LEU A 105 | 54.090 | 22.822 | 17.272 | 1.00 | 15.52 | A |
| ATOM | 820 | CB | LEU A 105 | 55.568 | 22.978 | 16.940 | 1.00 | 15.73 | A |
| ATOM | 821 | CG | LEU A 105 | 56.058 | 24.391 | 16.649 | 1.00 | 20.75 | A |
| ATOM | 822 | CD1 | LEU A 105 | 57.400 | 24.298 | 15.919 | 1.00 | 20.19 | A |
| ATOM | 823 | CD2 | LEU A 105 | 55.030 | 25.141 | 15.791 | 1.00 | 21.31 | A |
| ATOM | 824 | C | LEU A 105 | 53.709 | 21.362 | 17.202 | 1.00 | 15.97 | A |
| ATOM | 825 | O | LEU A 105 | 53.968 | 20.589 | 18.133 | 1.00 | 14.11 | A |
| ATOM | 826 | N | ILE A 106 | 53.078 | 20.993 | 16.099 | 1.00 | 14.18 | A |
| ATOM | 827 | CA | ILE A 106 | 52.643 | 19.630 | 15.903 | 1.00 | 15.40 | A |
| ATOM | 828 | CB | ILE A 106 | 51.122 | 19.576 | 15.636 | 1.00 | 15.11 | A |
| ATOM | 829 | CG2 | ILE A 106 | 50.661 | 18.135 | 15.592 | 1.00 | 12.46 | A |
| ATOM | 830 | CG1 | ILE A 106 | 50.380 | 20.354 | 16.734 | 1.00 | 15.51 | A |
| ATOM | 831 | CD1 | ILE A 106 | 48.862 | 20.413 | 16.565 | 1.00 | 12.83 | A |
| ATOM | 832 | C | ILE A 106 | 53.381 | 19.011 | 14.725 | 1.00 | 16.48 | A |
| ATOM | 833 | O | ILE A 106 | 53.484 | 19.607 | 13.651 | 1.00 | 17.37 | A |
| ATOM | 834 | N | CYS A 107 | 53.900 | 17.811 | 14.944 | 1.00 | 17.86 | A |
| ATOM | 835 | CA | CYS A 107 | 54.621 | 17.083 | 13.917 | 1.00 | 18.32 | A |
| ATOM | 836 | C | CYS A 107 | 53.886 | 15.776 | 13.663 | 1.00 | 18.29 | A |
| ATOM | 837 | O | CYS A 107 | 53.846 | 14.909 | 14.533 | 1.00 | 18.13 | A |
| ATOM | 838 | CB | CYS A 107 | 56.041 | 16.792 | 14.382 | 1.00 | 19.33 | A |
| ATOM | 839 | SG | CYS A 107 | 57.029 | 15.889 | 13.158 | 1.00 | 25.82 | A |
| ATOM | 840 | N | LEU A 108 | 53.304 | 15.649 | 12.472 | 1.00 | 17.89 | A |
| ATOM | 841 | CA | LEU A 108 | 52.556 | 14.456 | 12.088 | 1.00 | 18.82 | A |
| ATOM | 842 | CB | LEU A 108 | 51.330 | 14.850 | 11.252 | 1.00 | 20.17 | A |
| ATOM | 843 | CG | LEU A 108 | 50.129 | 13.900 | 11.053 | 1.00 | 21.48 | A |
| ATOM | 844 | CD1 | LEU A 108 | 49.623 | 14.049 | 9.624 | 1.00 | 20.62 | A |
| ATOM | 845 | CD2 | LEU A 108 | 50.493 | 12.458 | 11.316 | 1.00 | 18.40 | A |
| ATOM | 846 | C | LEU A 108 | 53.445 | 13.538 | 11.252 | 1.00 | 19.49 | A |
| ATOM | 847 | O | LEU A 108 | 53.841 | 13.892 | 10.144 | 1.00 | 20.39 | A |
| ATOM | 848 | N | VAL A 109 | 53.760 | 12.368 | 11.789 | 1.00 | 18.45 | A |
| ATOM | 849 | CA | VAL A 109 | 54.586 | 11.398 | 11.087 | 1.00 | 19.04 | A |
| ATOM | 850 | CB | VAL A 109 | 55.665 | 10.805 | 12.042 | 1.00 | 18.71 | A |
| ATOM | 851 | CG1 | VAL A 109 | 56.626 | 9.923 | 11.279 | 1.00 | 15.16 | A |
| ATOM | 852 | CG2 | VAL A 109 | 56.431 | 11.949 | 12.729 | 1.00 | 17.68 | A |
| ATOM | 853 | C | VAL A 109 | 53.611 | 10.322 | 10.606 | 1.00 | 20.50 | A |
| ATOM | 854 | O | VAL A 109 | 53.115 | 9.516 | 11.393 | 1.00 | 21.55 | A |
| ATOM | 855 | N | ASP A 110 | 53.326 | 10.337 | 9.308 | 1.00 | 21.50 | A |
| ATOM | 856 | CA | ASP A 110 | 52.376 | 9.407 | 8.700 | 1.00 | 21.95 | A |
| ATOM | 857 | CB | ASP A 110 | 51.493 | 10.165 | 7.701 | 1.00 | 22.25 | A |
| ATOM | 858 | CG | ASP A 110 | 50.084 | 9.612 | 7.622 | 1.00 | 24.20 | A |
| ATOM | 859 | OD1 | ASP A 110 | 49.874 | 8.435 | 7.989 | 1.00 | 23.87 | A |
| ATOM | 860 | OD2 | ASP A 110 | 49.182 | 10.356 | 7.182 | 1.00 | 25.94 | A |
| ATOM | 861 | C | ASP A 110 | 53.059 | 8.240 | 7.985 | 1.00 | 21.53 | A |
| ATOM | 862 | O | ASP A 110 | 54.273 | 8.254 | 7.782 | 1.00 | 18.80 | A |
| ATOM | 863 | N | ASN A 111 | 52.254 | 7.245 | 7.603 | 1.00 | 23.78 | A |
| ATOM | 864 | CA | ASN A 111 | 52.706 | 6.037 | 6.900 | 1.00 | 23.32 | A |
| ATOM | 865 | CB | ASN A 111 | 53.046 | 6.360 | 5.437 | 1.00 | 24.67 | A |
| ATOM | 866 | CG | ASN A 111 | 53.181 | 5.102 | 4.575 | 1.00 | 31.76 | A |
| ATOM | 867 | OD1 | ASN A 111 | 52.291 | 4.240 | 4.567 | 1.00 | 31.05 | A |
| ATOM | 868 | ND2 | ASN A 111 | 54.292 | 4.994 | 3.842 | 1.00 | 29.09 | A |
| ATOM | 869 | C | ASN A 111 | 53.905 | 5.389 | 7.587 | 1.00 | 23.68 | A |
| ATOM | 870 | O | ASN A 111 | 54.953 | 5.156 | 6.976 | 1.00 | 22.88 | A |
| ATOM | 871 | N | ILE A 112 | 53.738 | 5.090 | 8.868 | 1.00 | 22.97 | A |
| ATOM | 872 | CA | ILE A 112 | 54.797 | 4.473 | 9.646 | 1.00 | 20.73 | A |
| ATOM | 873 | CB | ILE A 112 | 54.791 | 4.967 | 11.108 | 1.00 | 20.13 | A |
| ATOM | 874 | CG2 | ILE A 112 | 55.979 | 4.363 | 11.864 | 1.00 | 15.53 | A |
| ATOM | 875 | CG1 | ILE A 112 | 54.833 | 6.495 | 11.158 | 1.00 | 19.14 | A |
| ATOM | 876 | CD1 | ILE A 112 | 54.671 | 7.058 | 12.575 | 1.00 | 20.42 | A |
| ATOM | 877 | C | ILE A 112 | 54.658 | 2.960 | 9.699 | 1.00 | 22.54 | A |
| ATOM | 878 | O | ILE A 112 | 53.605 | 2.436 | 10.054 | 1.00 | 22.65 | A |
| ATOM | 879 | N | PHE A 113 | 55.732 | 2.266 | 9.343 | 1.00 | 21.37 | A |
| ATOM | 880 | CA | PHE A 113 | 55.769 | 0.819 | 9.412 | 1.00 | 21.74 | A |
| ATOM | 881 | CB | PHE A 113 | 54.742 | 0.167 | 8.483 | 1.00 | 21.64 | A |
| ATOM | 882 | CG | PHE A 113 | 54.451 | -1.252 | 8.850 | 1.00 | 21.22 | A |
| ATOM | 883 | CD1 | PHE A 113 | 53.528 | -1.543 | 9.856 | 1.00 | 20.25 | A |

| ATOM | 884 | CD2 | PHE | A | 113 | 55.183 | -2.296 | 8.285 | 1.00 | 20.76 | A |
|------|-----|-----|-----|---|-----|--------|--------|-------|------|-------|---|
| ATOM | 885 | CE1 | PHE | A | 113 | 53.341 | -2.848 | 10.302 | 1.00 | 19.85 | A |
| ATOM | 886 | CE2 | PHE | A | 113 | 55.008 | -3.607 | 8.721 | 1.00 | 20.75 | A |
| ATOM | 887 | CZ | PHE | A | 113 | 54.086 | -3.887 | 9.735 | 1.00 | 21.24 | A |
| ATOM | 888 | C | PHE | A | 113 | 57.157 | 0.329 | 9.042 | 1.00 | 21.21 | A |
| ATOM | 889 | O | PHE | A | 113 | 57.700 | 0.719 | 8.011 | 1.00 | 19.97 | A |
| ATOM | 890 | N | PRO | A | 114 | 57.765 | -0.509 | 9.893 | 1.00 | 22.22 | A |
| ATOM | 891 | CD | PRO | A | 114 | 59.118 | -1.018 | 9.614 | 1.00 | 22.88 | A |
| ATOM | 892 | CA | PRO | A | 114 | 57.263 | -1.040 | 11.170 | 1.00 | 23.38 | A |
| ATOM | 893 | CB | PRO | A | 114 | 58.340 | -2.045 | 11.571 | 1.00 | 23.68 | A |
| ATOM | 894 | CG | PRO | A | 114 | 59.592 | -1.435 | 10.984 | 1.00 | 23.26 | A |
| ATOM | 895 | C | PRO | A | 114 | 57.078 | 0.059 | 12.221 | 1.00 | 24.33 | A |
| ATOM | 896 | O | PRO | A | 114 | 57.571 | 1.174 | 12.054 | 1.00 | 24.35 | A |
| ATOM | 897 | N | PRO | A | 115 | 56.363 | -0.247 | 13.319 | 1.00 | 24.59 | A |
| ATOM | 898 | CD | PRO | A | 115 | 55.579 | -1.472 | 13.567 | 1.00 | 22.60 | A |
| ATOM | 899 | CA | PRO | A | 115 | 56.135 | 0.751 | 14.372 | 1.00 | 23.79 | A |
| ATOM | 900 | CB | PRO | A | 115 | 54.923 | 0.194 | 15.107 | 1.00 | 23.96 | A |
| ATOM | 901 | CG | PRO | A | 115 | 55.129 | -1.291 | 14.998 | 1.00 | 23.45 | A |
| ATOM | 902 | C | PRO | A | 115 | 57.337 | 0.996 | 15.289 | 1.00 | 24.97 | A |
| ATOM | 903 | O | PRO | A | 115 | 57.322 | 0.670 | 16.482 | 1.00 | 23.11 | A |
| ATOM | 904 | N | VAL | A | 116 | 58.380 | 1.573 | 14.705 | 1.00 | 24.77 | A |
| ATOM | 905 | CA | VAL | A | 116 | 59.607 | 1.902 | 15.423 | 1.00 | 24.05 | A |
| ATOM | 906 | CB | VAL | A | 116 | 60.733 | 0.881 | 15.135 | 1.00 | 26.45 | A |
| ATOM | 907 | CG1 | VAL | A | 116 | 61.977 | 1.250 | 15.933 | 1.00 | 24.89 | A |
| ATOM | 908 | CG2 | VAL | A | 116 | 60.267 | -0.539 | 15.470 | 1.00 | 26.43 | A |
| ATOM | 909 | C | VAL | A | 116 | 60.043 | 3.254 | 14.875 | 1.00 | 24.47 | A |
| ATOM | 910 | O | VAL | A | 116 | 60.340 | 3.381 | 13.684 | 1.00 | 23.94 | A |
| ATOM | 911 | N | VAL | A | 117 | 60.088 | 4.269 | 15.728 | 1.00 | 22.43 | A |
| ATOM | 912 | CA | VAL | A | 117 | 60.472 | 5.577 | 15.239 | 1.00 | 22.18 | A |
| ATOM | 913 | CB | VAL | A | 117 | 59.247 | 6.277 | 14.565 | 1.00 | 21.24 | A |
| ATOM | 914 | CG1 | VAL | A | 117 | 58.276 | 6.807 | 15.631 | 1.00 | 17.87 | A |
| ATOM | 915 | CG2 | VAL | A | 117 | 59.710 | 7.387 | 13.653 | 1.00 | 19.98 | A |
| ATOM | 916 | C | VAL | A | 117 | 61.035 | 6.484 | 16.326 | 1.00 | 23.40 | A |
| ATOM | 917 | O | VAL | A | 117 | 60.743 | 6.323 | 17.512 | 1.00 | 22.77 | A |
| ATOM | 918 | N | ASN | A | 118 | 61.868 | 7.427 | 15.909 | 1.00 | 24.87 | A |
| ATOM | 919 | CA | ASN | A | 118 | 62.434 | 8.398 | 16.833 | 1.00 | 25.96 | A |
| ATOM | 920 | CB | ASN | A | 118 | 63.970 | 8.341 | 16.858 | 1.00 | 29.36 | A |
| ATOM | 921 | CG | ASN | A | 118 | 64.506 | 7.213 | 17.728 | 1.00 | 31.24 | A |
| ATOM | 922 | OD1 | ASN | A | 118 | 63.885 | 6.833 | 18.722 | 1.00 | 34.20 | A |
| ATOM | 923 | ND2 | ASN | A | 118 | 65.679 | 6.694 | 17.374 | 1.00 | 34.04 | A |
| ATOM | 924 | C | ASN | A | 118 | 61.989 | 9.746 | 16.312 | 1.00 | 24.87 | A |
| ATOM | 925 | O | ASN | A | 118 | 62.298 | 10.112 | 15.177 | 1.00 | 26.17 | A |
| ATOM | 926 | N | ILE | A | 119 | 61.229 | 10.468 | 17.122 | 1.00 | 23.82 | A |
| ATOM | 927 | CA | ILE | A | 119 | 60.774 | 11.793 | 16.727 | 1.00 | 23.07 | A |
| ATOM | 928 | CB | ILE | A | 119 | 59.231 | 11.892 | 16.711 | 1.00 | 22.65 | A |
| ATOM | 929 | CG2 | ILE | A | 119 | 58.797 | 13.197 | 16.051 | 1.00 | 18.01 | A |
| ATOM | 930 | CG1 | ILE | A | 119 | 58.642 | 10.716 | 15.936 | 1.00 | 21.02 | A |
| ATOM | 931 | CD1 | ILE | A | 119 | 57.135 | 10.714 | 15.921 | 1.00 | 21.88 | A |
| ATOM | 932 | C | ILE | A | 119 | 61.323 | 12.771 | 17.754 | 1.00 | 22.76 | A |
| ATOM | 933 | O | ILE | A | 119 | 61.013 | 12.680 | 18.940 | 1.00 | 22.92 | A |
| ATOM | 934 | N | THR | A | 120 | 62.162 | 13.691 | 17.303 | 1.00 | 23.11 | A |
| ATOM | 935 | CA | THR | A | 120 | 62.737 | 14.673 | 18.205 | 1.00 | 23.65 | A |
| ATOM | 936 | CB | THR | A | 120 | 64.216 | 14.363 | 18.495 | 1.00 | 25.23 | A |
| ATOM | 937 | OG1 | THR | A | 120 | 64.921 | 14.199 | 17.258 | 1.00 | 26.55 | A |
| ATOM | 938 | CG2 | THR | A | 120 | 64.335 | 13.081 | 19.331 | 1.00 | 23.93 | A |
| ATOM | 939 | C | THR | A | 120 | 62.622 | 16.064 | 17.616 | 1.00 | 23.20 | A |
| ATOM | 940 | O | THR | A | 120 | 62.437 | 16.232 | 16.412 | 1.00 | 23.15 | A |
| ATOM | 941 | N | TRP | A | 121 | 62.725 | 17.069 | 18.470 | 1.00 | 22.54 | A |
| ATOM | 942 | CA | TRP | A | 121 | 62.619 | 18.432 | 17.998 | 1.00 | 21.37 | A |
| ATOM | 943 | CB | TRP | A | 121 | 61.563 | 19.196 | 18.791 | 1.00 | 19.43 | A |
| ATOM | 944 | CG | TRP | A | 121 | 60.173 | 18.679 | 18.616 | 1.00 | 18.76 | A |
| ATOM | 945 | CD2 | TRP | A | 121 | 59.191 | 19.179 | 17.703 | 1.00 | 19.96 | A |
| ATOM | 946 | CE2 | TRP | A | 121 | 58.002 | 18.454 | 17.931 | 1.00 | 18.06 | A |
| ATOM | 947 | CE3 | TRP | A | 121 | 59.200 | 20.178 | 16.715 | 1.00 | 16.07 | A |
| ATOM | 948 | CD1 | TRP | A | 121 | 59.567 | 17.694 | 19.330 | 1.00 | 18.18 | A |
| ATOM | 949 | NE1 | TRP | A | 121 | 58.261 | 17.553 | 18.929 | 1.00 | 19.21 | A |
| ATOM | 950 | CZ2 | TRP | A | 121 | 56.827 | 18.694 | 17.210 | 1.00 | 16.20 | A |
| ATOM | 951 | CZ3 | TRP | A | 121 | 58.036 | 20.419 | 16.000 | 1.00 | 16.43 | A |
| ATOM | 952 | CH2 | TRP | A | 121 | 56.864 | 19.679 | 16.252 | 1.00 | 17.37 | A |
| ATOM | 953 | C | TRP | A | 121 | 63.927 | 19.178 | 18.097 | 1.00 | 22.88 | A |
| ATOM | 954 | O | TRP | A | 121 | 64.743 | 18.937 | 18.992 | 1.00 | 22.75 | A |
| ATOM | 955 | N | LEU | A | 122 | 64.109 | 20.100 | 17.164 | 1.00 | 23.24 | A |
| ATOM | 956 | CA | LEU | A | 122 | 65.291 | 20.930 | 17.136 | 1.00 | 22.66 | A |
| ATOM | 957 | CB | LEU | A | 122 | 66.094 | 20.699 | 15.850 | 1.00 | 23.05 | A |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 958 | CG | LEU | A | 122 | 66.638 | 19.293 | 15.563 | 1.00 | 22.23 | A |
| ATOM | 959 | CD1 | LEU | A | 122 | 67.404 | 19.326 | 14.253 | 1.00 | 20.93 | A |
| ATOM | 960 | CD2 | LEU | A | 122 | 67.542 | 18.830 | 16.700 | 1.00 | 20.21 | A |
| ATOM | 961 | C | LEU | A | 122 | 64.837 | 22.376 | 17.186 | 1.00 | 23.52 | A |
| ATOM | 962 | O | LEU | A | 122 | 63.830 | 22.752 | 16.572 | 1.00 | 21.74 | A |
| ATOM | 963 | N | SER | A | 123 | 65.579 | 23.174 | 17.945 | 1.00 | 23.69 | A |
| ATOM | 964 | CA | SER | A | 123 | 65.330 | 24.597 | 18.063 | 1.00 | 24.10 | A |
| ATOM | 965 | CB | SER | A | 123 | 64.998 | 24.983 | 19.504 | 1.00 | 25.22 | A |
| ATOM | 966 | OG | SER | A | 123 | 64.735 | 26.373 | 19.591 | 1.00 | 25.55 | A |
| ATOM | 967 | C | SER | A | 123 | 66.664 | 25.200 | 17.650 | 1.00 | 24.79 | A |
| ATOM | 968 | O | SER | A | 123 | 67.670 | 25.014 | 18.335 | 1.00 | 23.07 | A |
| ATOM | 969 | N | ASN | A | 124 | 66.666 | 25.903 | 16.521 | 1.00 | 25.02 | A |
| ATOM | 970 | CA | ASN | A | 124 | 67.880 | 26.513 | 15.986 | 1.00 | 25.63 | A |
| ATOM | 971 | CB | ASN | A | 124 | 68.351 | 27.676 | 16.868 | 1.00 | 24.46 | A |
| ATOM | 972 | CG | ASN | A | 124 | 67.376 | 28.839 | 16.873 | 1.00 | 25.33 | A |
| ATOM | 973 | OD1 | ASN | A | 124 | 66.636 | 29.056 | 15.907 | 1.00 | 26.04 | A |
| ATOM | 974 | ND2 | ASN | A | 124 | 67.381 | 29.606 | 17.956 | 1.00 | 21.77 | A |
| ATOM | 975 | C | ASN | A | 124 | 69.006 | 25.487 | 15.838 | 1.00 | 26.53 | A |
| ATOM | 976 | O | ASN | A | 124 | 70.132 | 25.706 | 16.301 | 1.00 | 26.36 | A |
| ATOM | 977 | N | GLY | A | 125 | 68.684 | 24.361 | 15.205 | 1.00 | 24.78 | A |
| ATOM | 978 | CA | GLY | A | 125 | 69.669 | 23.326 | 14.964 | 1.00 | 26.09 | A |
| ATOM | 979 | C | GLY | A | 125 | 70.030 | 22.377 | 16.089 | 1.00 | 27.35 | A |
| ATOM | 980 | O | GLY | A | 125 | 70.728 | 21.395 | 15.846 | 1.00 | 28.21 | A |
| ATOM | 981 | N | HIS | A | 126 | 69.566 | 22.645 | 17.307 | 1.00 | 28.65 | A |
| ATOM | 982 | CA | HIS | A | 126 | 69.889 | 21.774 | 18.430 | 1.00 | 30.12 | A |
| ATOM | 983 | CB | HIS | A | 126 | 70.816 | 22.507 | 19.408 | 1.00 | 32.68 | A |
| ATOM | 984 | CG | HIS | A | 126 | 70.226 | 23.750 | 19.996 | 1.00 | 35.25 | A |
| ATOM | 985 | CD2 | HIS | A | 126 | 70.296 | 25.044 | 19.601 | 1.00 | 36.90 | A |
| ATOM | 986 | ND1 | HIS | A | 126 | 69.475 | 23.743 | 21.151 | 1.00 | 35.93 | A |
| ATOM | 987 | CE1 | HIS | A | 126 | 69.110 | 24.979 | 21.445 | 1.00 | 36.88 | A |
| ATOM | 988 | NE2 | HIS | A | 126 | 69.595 | 25.788 | 20.520 | 1.00 | 36.73 | A |
| ATOM | 989 | C | HIS | A | 126 | 68.661 | 21.220 | 19.149 | 1.00 | 30.87 | A |
| ATOM | 990 | O | HIS | A | 126 | 67.634 | 21.889 | 19.270 | 1.00 | 31.49 | A |
| ATOM | 991 | N | SER | A | 127 | 68.789 | 19.990 | 19.635 | 1.00 | 30.93 | A |
| ATOM | 992 | CA | SER | A | 127 | 67.697 | 19.286 | 20.302 | 1.00 | 33.08 | A |
| ATOM | 993 | CB | SER | A | 127 | 68.165 | 17.889 | 20.714 | 1.00 | 33.91 | A |
| ATOM | 994 | OG | SER | A | 127 | 69.231 | 17.979 | 21.645 | 1.00 | 38.34 | A |
| ATOM | 995 | C | SER | A | 127 | 67.050 | 19.971 | 21.501 | 1.00 | 32.98 | A |
| ATOM | 996 | O | SER | A | 127 | 67.708 | 20.654 | 22.288 | 1.00 | 34.83 | A |
| ATOM | 997 | N | VAL | A | 128 | 65.743 | 19.770 | 21.624 | 1.00 | 32.42 | A |
| ATOM | 998 | CA | VAL | A | 128 | 64.960 | 20.325 | 22.716 | 1.00 | 31.29 | A |
| ATOM | 999 | CB | VAL | A | 128 | 63.645 | 20.921 | 22.202 | 1.00 | 30.48 | A |
| ATOM | 1000 | CG1 | VAL | A | 128 | 62.856 | 21.520 | 23.358 | 1.00 | 27.06 | A |
| ATOM | 1001 | CG2 | VAL | A | 128 | 63.937 | 21.970 | 21.142 | 1.00 | 28.52 | A |
| ATOM | 1002 | C | VAL | A | 128 | 64.645 | 19.183 | 23.669 | 1.00 | 32.28 | A |
| ATOM | 1003 | O | VAL | A | 128 | 64.275 | 18.093 | 23.237 | 1.00 | 32.80 | A |
| ATOM | 1004 | N | THR | A | 129 | 64.786 | 19.437 | 24.965 | 1.00 | 33.30 | A |
| ATOM | 1005 | CA | THR | A | 129 | 64.546 | 18.411 | 25.981 | 1.00 | 33.70 | A |
| ATOM | 1006 | CB | THR | A | 129 | 65.740 | 18.344 | 26.966 | 1.00 | 34.52 | A |
| ATOM | 1007 | OG1 | THR | A | 129 | 65.969 | 19.643 | 27.528 | 1.00 | 38.18 | A |
| ATOM | 1008 | CG2 | THR | A | 129 | 67.006 | 17.898 | 26.245 | 1.00 | 34.60 | A |
| ATOM | 1009 | C | THR | A | 129 | 63.257 | 18.591 | 26.791 | 1.00 | 32.08 | A |
| ATOM | 1010 | O | THR | A | 129 | 62.645 | 17.615 | 27.220 | 1.00 | 34.04 | A |
| ATOM | 1011 | N | GLU | A | 130 | 62.843 | 19.835 | 26.993 | 1.00 | 28.85 | A |
| ATOM | 1012 | CA | GLU | A | 130 | 61.639 | 20.119 | 27.762 | 1.00 | 26.09 | A |
| ATOM | 1013 | CB | GLU | A | 130 | 61.926 | 21.236 | 28.770 | 1.00 | 28.58 | A |
| ATOM | 1014 | CG | GLU | A | 130 | 62.962 | 20.894 | 29.822 | 1.00 | 32.87 | A |
| ATOM | 1015 | CD | GLU | A | 130 | 62.592 | 19.654 | 30.609 | 1.00 | 35.34 | A |
| ATOM | 1016 | OE1 | GLU | A | 130 | 61.392 | 19.475 | 30.907 | 1.00 | 37.85 | A |
| ATOM | 1017 | OE2 | GLU | A | 130 | 63.501 | 18.865 | 30.941 | 1.00 | 36.29 | A |
| ATOM | 1018 | C | GLU | A | 130 | 60.451 | 20.534 | 26.893 | 1.00 | 23.53 | A |
| ATOM | 1019 | O | GLU | A | 130 | 60.629 | 21.166 | 25.859 | 1.00 | 19.76 | A |
| ATOM | 1020 | N | GLY | A | 131 | 59.243 | 20.188 | 27.334 | 1.00 | 21.13 | A |
| ATOM | 1021 | CA | GLY | A | 131 | 58.046 | 20.563 | 26.601 | 1.00 | 20.14 | A |
| ATOM | 1022 | C | GLY | A | 131 | 57.693 | 19.684 | 25.421 | 1.00 | 20.64 | A |
| ATOM | 1023 | O | GLY | A | 131 | 56.989 | 20.109 | 24.507 | 1.00 | 20.11 | A |
| ATOM | 1024 | N | VAL | A | 132 | 58.164 | 18.447 | 25.444 | 1.00 | 18.28 | A |
| ATOM | 1025 | CA | VAL | A | 132 | 57.899 | 17.527 | 24.355 | 1.00 | 20.08 | A |
| ATOM | 1026 | CB | VAL | A | 132 | 59.230 | 16.985 | 23.767 | 1.00 | 20.35 | A |
| ATOM | 1027 | CG1 | VAL | A | 132 | 58.946 | 15.874 | 22.772 | 1.00 | 22.11 | A |
| ATOM | 1028 | CG2 | VAL | A | 132 | 60.006 | 18.114 | 23.093 | 1.00 | 20.17 | A |
| ATOM | 1029 | C | VAL | A | 132 | 57.027 | 16.340 | 24.786 | 1.00 | 20.06 | A |
| ATOM | 1030 | O | VAL | A | 132 | 57.194 | 15.794 | 25.875 | 1.00 | 18.65 | A |
| ATOM | 1031 | N | SER | A | 133 | 56.094 | 15.948 | 23.925 | 1.00 | 17.90 | A |

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| ATOM | 1032 | CA | SER A 133 | 55.238 | 14.802 | 24.215 | 1.00 | 18.16 | A |
| ATOM | 1033 | CB | SER A 133 | 54.045 | 15.206 | 25.094 | 1.00 | 18.24 | A |
| ATOM | 1034 | OG | SER A 133 | 53.202 | 16.143 | 24.440 | 1.00 | 24.24 | A |
| ATOM | 1035 | C | SER A 133 | 54.738 | 14.200 | 22.914 | 1.00 | 16.52 | A |
| ATOM | 1036 | O | SER A 133 | 54.876 | 14.794 | 21.843 | 1.00 | 16.18 | A |
| ATOM | 1037 | N | GLU A 134 | 54.166 | 13.009 | 22.996 | 1.00 | 17.45 | A |
| ATOM | 1038 | CA | GLU A 134 | 53.653 | 12.369 | 21.800 | 1.00 | 18.50 | A |
| ATOM | 1039 | CB | GLU A 134 | 54.797 | 11.661 | 21.050 | 1.00 | 22.31 | A |
| ATOM | 1040 | CG | GLU A 134 | 55.475 | 10.513 | 21.801 | 1.00 | 24.62 | A |
| ATOM | 1041 | CD | GLU A 134 | 56.610 | 9.859 | 20.992 | 1.00 | 28.65 | A |
| ATOM | 1042 | OE1 | GLU A 134 | 56.932 | 8.680 | 21.254 | 1.00 | 29.58 | A |
| ATOM | 1043 | OE2 | GLU A 134 | 57.188 | 10.521 | 20.099 | 1.00 | 27.96 | A |
| ATOM | 1044 | C | GLU A 134 | 52.523 | 11.389 | 22.087 | 1.00 | 18.44 | A |
| ATOM | 1045 | O | GLU A 134 | 52.279 | 11.003 | 23.234 | 1.00 | 17.30 | A |
| ATOM | 1046 | N | THR A 135 | 51.824 | 11.008 | 21.027 | 1.00 | 16.71 | A |
| ATOM | 1047 | CA | THR A 135 | 50.733 | 10.059 | 21.119 | 1.00 | 15.49 | A |
| ATOM | 1048 | CB | THR A 135 | 49.738 | 10.246 | 19.967 | 1.00 | 16.16 | A |
| ATOM | 1049 | OG1 | THR A 135 | 50.369 | 9.867 | 18.731 | 1.00 | 16.02 | A |
| ATOM | 1050 | CG2 | THR A 135 | 49.280 | 11.697 | 19.879 | 1.00 | 14.19 | A |
| ATOM | 1051 | C | THR A 135 | 51.346 | 8.682 | 20.946 | 1.00 | 17.19 | A |
| ATOM | 1052 | O | THR A 135 | 52.551 | 8.554 | 20.733 | 1.00 | 17.26 | A |
| ATOM | 1053 | N | SER A 136 | 50.519 | 7.650 | 21.047 | 1.00 | 17.53 | A |
| ATOM | 1054 | CA | SER A 136 | 51.001 | 6.297 | 20.818 | 1.00 | 15.92 | A |
| ATOM | 1055 | CB | SER A 136 | 50.035 | 5.266 | 21.416 | 1.00 | 16.85 | A |
| ATOM | 1056 | OG | SER A 136 | 49.756 | 5.532 | 22.781 | 1.00 | 18.22 | A |
| ATOM | 1057 | C | SER A 136 | 50.967 | 6.187 | 19.294 | 1.00 | 15.84 | A |
| ATOM | 1058 | O | SER A 136 | 50.715 | 7.169 | 18.596 | 1.00 | 17.25 | A |
| ATOM | 1059 | N | PHE A 137 | 51.236 | 5.003 | 18.767 | 1.00 | 17.08 | A |
| ATOM | 1060 | CA | PHE A 137 | 51.155 | 4.806 | 17.333 | 1.00 | 15.67 | A |
| ATOM | 1061 | CB | PHE A 137 | 51.874 | 3.519 | 16.936 | 1.00 | 13.47 | A |
| ATOM | 1062 | CG | PHE A 137 | 53.363 | 3.628 | 16.951 | 1.00 | 14.48 | A |
| ATOM | 1063 | CD1 | PHE A 137 | 54.037 | 4.255 | 15.907 | 1.00 | 15.82 | A |
| ATOM | 1064 | CD2 | PHE A 137 | 54.100 | 3.112 | 18.010 | 1.00 | 15.21 | A |
| ATOM | 1065 | CE1 | PHE A 137 | 55.427 | 4.367 | 15.918 | 1.00 | 15.72 | A |
| ATOM | 1066 | CE2 | PHE A 137 | 55.490 | 3.220 | 18.031 | 1.00 | 15.14 | A |
| ATOM | 1067 | CZ | PHE A 137 | 56.152 | 3.848 | 16.983 | 1.00 | 14.35 | A |
| ATOM | 1068 | C | PHE A 137 | 49.659 | 4.657 | 17.067 | 1.00 | 16.21 | A |
| ATOM | 1069 | O | PHE A 137 | 49.037 | 3.767 | 17.622 | 1.00 | 18.05 | A |
| ATOM | 1070 | N | LEU A 138 | 49.074 | 5.534 | 16.259 | 1.00 | 17.51 | A |
| ATOM | 1071 | CA | LEU A 138 | 47.648 | 5.433 | 15.953 | 1.00 | 19.20 | A |
| ATOM | 1072 | CB | LEU A 138 | 47.017 | 6.822 | 15.800 | 1.00 | 20.80 | A |
| ATOM | 1073 | CG | LEU A 138 | 46.809 | 7.688 | 17.044 | 1.00 | 23.47 | A |
| ATOM | 1074 | CD1 | LEU A 138 | 46.141 | 6.879 | 18.144 | 1.00 | 24.75 | A |
| ATOM | 1075 | CD2 | LEU A 138 | 48.140 | 8.212 | 17.529 | 1.00 | 27.62 | A |
| ATOM | 1076 | C | LEU A 138 | 47.490 | 4.637 | 14.658 | 1.00 | 18.41 | A |
| ATOM | 1077 | O | LEU A 138 | 48.218 | 4.862 | 13.698 | 1.00 | 16.16 | A |
| ATOM | 1078 | N | SER A 139 | 46.530 | 3.716 | 14.630 | 1.00 | 18.51 | A |
| ATOM | 1079 | CA | SER A 139 | 46.333 | 2.863 | 13.460 | 1.00 | 17.61 | A |
| ATOM | 1080 | CB | SER A 139 | 45.481 | 1.656 | 13.836 | 1.00 | 18.17 | A |
| ATOM | 1081 | OG | SER A 139 | 44.134 | 2.036 | 14.040 | 1.00 | 20.80 | A |
| ATOM | 1082 | C | SER A 139 | 45.729 | 3.510 | 12.216 | 1.00 | 17.44 | A |
| ATOM | 1083 | O | SER A 139 | 45.122 | 4.578 | 12.276 | 1.00 | 16.41 | A |
| ATOM | 1084 | N | LYS A 140 | 45.908 | 2.822 | 11.088 | 1.00 | 18.56 | A |
| ATOM | 1085 | CA | LYS A 140 | 45.402 | 3.237 | 9.778 | 1.00 | 18.37 | A |
| ATOM | 1086 | CB | LYS A 140 | 46.543 | 3.751 | 8.895 | 1.00 | 21.60 | A |
| ATOM | 1087 | CG | LYS A 140 | 47.149 | 5.085 | 9.326 | 1.00 | 24.86 | A |
| ATOM | 1088 | CD | LYS A 140 | 46.513 | 6.267 | 8.602 | 1.00 | 30.27 | A |
| ATOM | 1089 | CE | LYS A 140 | 46.961 | 6.345 | 7.150 | 1.00 | 29.93 | A |
| ATOM | 1090 | NZ | LYS A 140 | 48.440 | 6.349 | 7.038 | 1.00 | 30.14 | A |
| ATOM | 1091 | C | LYS A 140 | 44.773 | 2.012 | 9.118 | 1.00 | 17.79 | A |
| ATOM | 1092 | O | LYS A 140 | 45.106 | 0.878 | 9.458 | 1.00 | 17.76 | A |
| ATOM | 1093 | N | SER A 141 | 43.882 | 2.234 | 8.160 | 1.00 | 18.54 | A |
| ATOM | 1094 | CA | SER A 141 | 43.220 | 1.124 | 7.481 | 1.00 | 21.55 | A |
| ATOM | 1095 | CB | SER A 141 | 42.047 | 1.634 | 6.630 | 1.00 | 21.05 | A |
| ATOM | 1096 | OG | SER A 141 | 42.490 | 2.482 | 5.588 | 1.00 | 28.41 | A |
| ATOM | 1097 | C | SER A 141 | 44.154 | 0.263 | 6.625 | 1.00 | 21.42 | A |
| ATOM | 1098 | O | SER A 141 | 43.828 | -0.885 | 6.332 | 1.00 | 21.49 | A |
| ATOM | 1099 | N | ASP A 142 | 45.311 | 0.793 | 6.226 | 1.00 | 20.12 | A |
| ATOM | 1100 | CA | ASP A 142 | 46.234 | -0.016 | 5.430 | 1.00 | 19.88 | A |
| ATOM | 1101 | CB | ASP A 142 | 47.008 | 0.843 | 4.420 | 1.00 | 22.82 | A |
| ATOM | 1102 | CG | ASP A 142 | 47.949 | 1.834 | 5.076 | 1.00 | 24.81 | A |
| ATOM | 1103 | OD1 | ASP A 142 | 47.837 | 2.061 | 6.298 | 1.00 | 25.33 | A |
| ATOM | 1104 | OD2 | ASP A 142 | 48.799 | 2.395 | 4.354 | 1.00 | 28.43 | A |
| ATOM | 1105 | C | ASP A 142 | 47.176 | -0.752 | 6.368 | 1.00 | 20.11 | A |

| ATOM | 1106 | O   | ASP A 142 | 48.127 | -1.416 | 5.946  | 1.00 | 19.21 | A |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1107 | N   | HIS A 143 | 46.885 | -0.626 | 7.659  | 1.00 | 18.99 | A |
| ATOM | 1108 | CA  | HIS A 143 | 47.637 | -1.295 | 8.706  | 1.00 | 17.27 | A |
| ATOM | 1109 | CB  | HIS A 143 | 47.686 | -2.792 | 8.409  | 1.00 | 16.45 | A |
| ATOM | 1110 | CG  | HIS A 143 | 46.329 | -3.396 | 8.190  | 1.00 | 18.33 | A |
| ATOM | 1111 | CD2 | HIS A 143 | 45.860 | -4.211 | 7.213  | 1.00 | 17.59 | A |
| ATOM | 1112 | ND1 | HIS A 143 | 45.262 | -3.151 | 9.032  | 1.00 | 15.97 | A |
| ATOM | 1113 | CE1 | HIS A 143 | 44.194 | -3.786 | 8.580  | 1.00 | 19.46 | A |
| ATOM | 1114 | NE2 | HIS A 143 | 44.529 | -4.436 | 7.478  | 1.00 | 18.06 | A |
| ATOM | 1115 | C   | HIS A 143 | 49.019 | -0.749 | 9.030  | 1.00 | 19.46 | A |
| ATOM | 1116 | O   | HIS A 143 | 49.812 | -1.401 | 9.715  | 1.00 | 19.95 | A |
| ATOM | 1117 | N   | SER A 144 | 49.301 | 0.454  | 8.536  | 1.00 | 19.70 | A |
| ATOM | 1118 | CA  | SER A 144 | 50.542 | 1.141  | 8.852  | 1.00 | 20.18 | A |
| ATOM | 1119 | CB  | SER A 144 | 51.018 | 2.011  | 7.678  | 1.00 | 19.91 | A |
| ATOM | 1120 | OG  | SER A 144 | 50.099 | 3.044  | 7.364  | 1.00 | 23.64 | A |
| ATOM | 1121 | C   | SER A 144 | 50.109 | 2.018  | 10.034 | 1.00 | 19.40 | A |
| ATOM | 1122 | O   | SER A 144 | 48.970 | 1.906  | 10.499 | 1.00 | 19.70 | A |
| ATOM | 1123 | N   | PHE A 145 | 50.986 | 2.883  | 10.525 | 1.00 | 16.99 | A |
| ATOM | 1124 | CA  | PHE A 145 | 50.614 | 3.728  | 11.649 | 1.00 | 16.06 | A |
| ATOM | 1125 | CB  | PHE A 145 | 51.325 | 3.274  | 12.929 | 1.00 | 16.25 | A |
| ATOM | 1126 | CG  | PHE A 145 | 51.062 | 1.841  | 13.297 | 1.00 | 19.53 | A |
| ATOM | 1127 | CD1 | PHE A 145 | 51.754 | 0.807  | 12.672 | 1.00 | 20.17 | A |
| ATOM | 1128 | CD2 | PHE A 145 | 50.114 | 1.522  | 14.263 | 1.00 | 18.18 | A |
| ATOM | 1129 | CE1 | PHE A 145 | 51.505 | -0.525 | 13.005 | 1.00 | 21.33 | A |
| ATOM | 1130 | CE2 | PHE A 145 | 49.856 | 0.193  | 14.606 | 1.00 | 19.50 | A |
| ATOM | 1131 | CZ  | PHE A 145 | 50.553 | -0.831 | 13.975 | 1.00 | 20.23 | A |
| ATOM | 1132 | C   | PHE A 145 | 50.955 | 5.182  | 11.419 | 1.00 | 15.69 | A |
| ATOM | 1133 | O   | PHE A 145 | 51.548 | 5.538  | 10.404 | 1.00 | 16.69 | A |
| ATOM | 1134 | N   | PHE A 146 | 50.530 | 6.021  | 12.357 | 1.00 | 14.53 | A |
| ATOM | 1135 | CA  | PHE A 146 | 50.869 | 7.429  | 12.332 | 1.00 | 16.67 | A |
| ATOM | 1136 | CB  | PHE A 146 | 49.841 | 8.279  | 11.552 | 1.00 | 16.59 | A |
| ATOM | 1137 | CG  | PHE A 146 | 48.535 | 8.528  | 12.259 | 1.00 | 15.25 | A |
| ATOM | 1138 | CD1 | PHE A 146 | 48.370 | 9.644  | 13.071 | 1.00 | 15.42 | A |
| ATOM | 1139 | CD2 | PHE A 146 | 47.433 | 7.708  | 12.019 | 1.00 | 16.06 | A |
| ATOM | 1140 | CE1 | PHE A 146 | 47.123 | 9.952  | 13.629 | 1.00 | 17.50 | A |
| ATOM | 1141 | CE2 | PHE A 146 | 46.180 | 8.003  | 12.571 | 1.00 | 16.80 | A |
| ATOM | 1142 | CZ  | PHE A 146 | 46.023 | 9.126  | 13.375 | 1.00 | 17.47 | A |
| ATOM | 1143 | C   | PHE A 146 | 51.017 | 7.841  | 13.783 | 1.00 | 17.00 | A |
| ATOM | 1144 | O   | PHE A 146 | 50.345 | 7.308  | 14.661 | 1.00 | 19.50 | A |
| ATOM | 1145 | N   | LYS A 147 | 51.950 | 8.747  | 14.032 | 1.00 | 17.82 | A |
| ATOM | 1146 | CA  | LYS A 147 | 52.224 | 9.221  | 15.377 | 1.00 | 18.67 | A |
| ATOM | 1147 | CB  | LYS A 147 | 53.540 | 8.604  | 15.863 | 1.00 | 20.48 | A |
| ATOM | 1148 | CG  | LYS A 147 | 53.771 | 8.668  | 17.359 | 1.00 | 25.54 | A |
| ATOM | 1149 | CD  | LYS A 147 | 54.822 | 7.645  | 17.774 | 1.00 | 29.96 | A |
| ATOM | 1150 | CE  | LYS A 147 | 54.835 | 7.417  | 19.282 | 1.00 | 30.05 | A |
| ATOM | 1151 | NZ  | LYS A 147 | 55.740 | 6.291  | 19.643 | 1.00 | 33.05 | A |
| ATOM | 1152 | C   | LYS A 147 | 52.315 | 10.743 | 15.338 | 1.00 | 17.25 | A |
| ATOM | 1153 | O   | LYS A 147 | 52.716 | 11.320 | 14.329 | 1.00 | 19.15 | A |
| ATOM | 1154 | N   | ILE A 148 | 51.932 | 11.391 | 16.428 | 1.00 | 15.47 | A |
| ATOM | 1155 | CA  | ILE A 148 | 51.969 | 12.846 | 16.494 | 1.00 | 14.99 | A |
| ATOM | 1156 | CB  | ILE A 148 | 50.529 | 13.424 | 16.642 | 1.00 | 15.37 | A |
| ATOM | 1157 | CG2 | ILE A 148 | 50.566 | 14.932 | 16.740 | 1.00 | 14.06 | A |
| ATOM | 1158 | CG1 | ILE A 148 | 49.689 | 13.025 | 15.426 | 1.00 | 16.41 | A |
| ATOM | 1159 | CD1 | ILE A 148 | 48.223 | 13.325 | 15.550 | 1.00 | 18.61 | A |
| ATOM | 1160 | C   | ILE A 148 | 52.829 | 13.271 | 17.682 | 1.00 | 17.07 | A |
| ATOM | 1161 | O   | ILE A 148 | 52.721 | 12.702 | 18.772 | 1.00 | 15.61 | A |
| ATOM | 1162 | N   | SER A 149 | 53.696 | 14.255 | 17.458 | 1.00 | 16.79 | A |
| ATOM | 1163 | CA  | SER A 149 | 54.570 | 14.757 | 18.514 | 1.00 | 17.66 | A |
| ATOM | 1164 | CB  | SER A 149 | 56.042 | 14.612 | 18.116 | 1.00 | 15.95 | A |
| ATOM | 1165 | OG  | SER A 149 | 56.900 | 14.956 | 19.190 | 1.00 | 17.31 | A |
| ATOM | 1166 | C   | SER A 149 | 54.239 | 16.225 | 18.763 | 1.00 | 18.34 | A |
| ATOM | 1167 | O   | SER A 149 | 53.854 | 16.949 | 17.842 | 1.00 | 18.33 | A |
| ATOM | 1168 | N   | TYR A 150 | 54.401 | 16.665 | 20.005 | 1.00 | 16.95 | A |
| ATOM | 1169 | CA  | TYR A 150 | 54.085 | 18.040 | 20.362 | 1.00 | 17.59 | A |
| ATOM | 1170 | CB  | TYR A 150 | 52.893 | 18.057 | 21.310 | 1.00 | 17.57 | A |
| ATOM | 1171 | CG  | TYR A 150 | 51.679 | 17.314 | 20.797 | 1.00 | 18.52 | A |
| ATOM | 1172 | CD1 | TYR A 150 | 50.879 | 17.851 | 19.789 | 1.00 | 17.12 | A |
| ATOM | 1173 | CE1 | TYR A 150 | 49.733 | 17.182 | 19.340 | 1.00 | 18.32 | A |
| ATOM | 1174 | CD2 | TYR A 150 | 51.313 | 16.078 | 21.345 | 1.00 | 18.89 | A |
| ATOM | 1175 | CE2 | TYR A 150 | 50.176 | 15.399 | 20.901 | 1.00 | 17.65 | A |
| ATOM | 1176 | CZ  | TYR A 150 | 49.391 | 15.957 | 19.900 | 1.00 | 17.92 | A |
| ATOM | 1177 | OH  | TYR A 150 | 48.275 | 15.285 | 19.457 | 1.00 | 19.69 | A |
| ATOM | 1178 | C   | TYR A 150 | 55.237 | 18.768 | 21.021 | 1.00 | 17.16 | A |
| ATOM | 1179 | O   | TYR A 150 | 55.953 | 18.207 | 21.847 | 1.00 | 19.65 | A |

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ATOM   1180  N   LEU A 151      55.409  20.029  20.649  1.00 17.01      A
ATOM   1181  CA  LEU A 151      56.449  20.868  21.224  1.00 15.24      A
ATOM   1182  CB  LEU A 151      57.540  21.182  20.197  1.00 16.33      A
ATOM   1183  CG  LEU A 151      58.487  22.335  20.575  1.00 16.27      A
ATOM   1184  CD1 LEU A 151      59.402  21.906  21.706  1.00 17.13      A
ATOM   1185  CD2 LEU A 151      59.315  22.755  19.359  1.00 19.34      A
ATOM   1186  C   LEU A 151      55.825  22.174  21.666  1.00 16.08      A
ATOM   1187  O   LEU A 151      55.221  22.881  20.860  1.00 16.22      A
ATOM   1188  N   THR A 152      55.952  22.497  22.945  1.00 16.84      A
ATOM   1189  CA  THR A 152      55.428  23.765  23.424  1.00 18.70      A
ATOM   1190  CB  THR A 152      55.283  23.799  24.946  1.00 20.14      A
ATOM   1191  OG1 THR A 152      56.576  23.633  25.544  1.00 23.32      A
ATOM   1192  CG2 THR A 152      54.355  22.694  25.419  1.00 18.36      A
ATOM   1193  C   THR A 152      56.498  24.772  23.050  1.00 20.04      A
ATOM   1194  O   THR A 152      57.689  24.448  23.034  1.00 20.72      A
ATOM   1195  N   LEU A 153      56.085  25.986  22.735  1.00 20.63      A
ATOM   1196  CA  LEU A 153      57.043  27.014  22.389  1.00 24.69      A
ATOM   1197  CB  LEU A 153      57.579  26.794  20.960  1.00 24.19      A
ATOM   1198  CG  LEU A 153      56.716  26.942  19.694  1.00 26.72      A
ATOM   1199  CD1 LEU A 153      55.303  26.451  19.959  1.00 27.32      A
ATOM   1200  CD2 LEU A 153      56.686  28.393  19.249  1.00 26.15      A
ATOM   1201  C   LEU A 153      56.410  28.385  22.531  1.00 26.36      A
ATOM   1202  O   LEU A 153      55.180  28.511  22.597  1.00 29.59      A
ATOM   1203  N   LEU A 154      57.262  29.401  22.620  1.00 26.29      A
ATOM   1204  CA  LEU A 154      56.830  30.787  22.729  1.00 26.89      A
ATOM   1205  CB  LEU A 154      57.459  31.444  23.965  1.00 26.94      A
ATOM   1206  CG  LEU A 154      56.966  32.833  24.407  1.00 28.58      A
ATOM   1207  CD1 LEU A 154      55.507  32.755  24.864  1.00 24.43      A
ATOM   1208  CD2 LEU A 154      57.845  33.342  25.549  1.00 27.14      A
ATOM   1209  C   LEU A 154      57.337  31.458  21.456  1.00 28.94      A
ATOM   1210  O   LEU A 154      58.538  31.689  21.304  1.00 30.73      A
ATOM   1211  N   PRO A 155      56.428  31.773  20.518  1.00 30.57      A
ATOM   1212  CD  PRO A 155      54.975  31.534  20.559  1.00 29.60      A
ATOM   1213  CA  PRO A 155      56.806  32.412  19.254  1.00 31.63      A
ATOM   1214  CB  PRO A 155      55.460  32.668  18.581  1.00 30.63      A
ATOM   1215  CG  PRO A 155      54.612  31.552  19.087  1.00 28.73      A
ATOM   1216  C   PRO A 155      57.639  33.688  19.370  1.00 33.58      A
ATOM   1217  O   PRO A 155      57.322  34.593  20.136  1.00 33.98      A
ATOM   1218  N   SER A 156      58.706  33.741  18.586  1.00 35.79      A
ATOM   1219  CA  SER A 156      59.595  34.888  18.546  1.00 37.77      A
ATOM   1220  CB  SER A 156      60.604  34.839  19.694  1.00 38.66      A
ATOM   1221  OG  SER A 156      59.955  34.966  20.949  1.00 44.00      A
ATOM   1222  C   SER A 156      60.332  34.841  17.222  1.00 38.83      A
ATOM   1223  O   SER A 156      60.257  33.849  16.492  1.00 38.36      A
ATOM   1224  N   ALA A 157      61.042  35.915  16.909  1.00 40.38      A
ATOM   1225  CA  ALA A 157      61.796  35.972  15.670  1.00 39.93      A
ATOM   1226  CB  ALA A 157      61.822  37.401  15.148  1.00 40.36      A
ATOM   1227  C   ALA A 157      63.214  35.466  15.918  1.00 39.65      A
ATOM   1228  O   ALA A 157      64.058  35.504  15.021  1.00 39.72      A
ATOM   1229  N   GLU A 158      63.463  34.984  17.135  1.00 39.12      A
ATOM   1230  CA  GLU A 158      64.784  34.480  17.517  1.00 40.24      A
ATOM   1231  CB  GLU A 158      65.082  34.808  18.988  1.00 44.21      A
ATOM   1232  CG  GLU A 158      65.426  36.268  19.287  1.00 50.31      A
ATOM   1233  CD  GLU A 158      64.204  37.174  19.356  1.00 55.36      A
ATOM   1234  OE1 GLU A 158      64.353  38.351  19.765  1.00 55.75      A
ATOM   1235  OE2 GLU A 158      63.095  36.712  19.002  1.00 58.12      A
ATOM   1236  C   GLU A 158      65.005  32.979  17.303  1.00 38.02      A
ATOM   1237  O   GLU A 158      66.130  32.493  17.419  1.00 36.30      A
ATOM   1238  N   GLU A 159      63.950  32.234  17.002  1.00 35.79      A
ATOM   1239  CA  GLU A 159      64.136  30.807  16.805  1.00 35.02      A
ATOM   1240  CB  GLU A 159      63.949  30.066  18.135  1.00 36.97      A
ATOM   1241  CG  GLU A 159      62.699  30.439  18.891  1.00 41.68      A
ATOM   1242  CD  GLU A 159      62.717  29.933  20.323  1.00 44.82      A
ATOM   1243  OE1 GLU A 159      62.819  28.705  20.527  1.00 46.62      A
ATOM   1244  OE2 GLU A 159      62.631  30.767  21.248  1.00 47.25      A
ATOM   1245  C   GLU A 159      63.277  30.162  15.735  1.00 32.21      A
ATOM   1246  O   GLU A 159      62.147  30.574  15.473  1.00 32.05      A
ATOM   1247  N   SER A 160      63.849  29.147  15.107  1.00 29.55      A
ATOM   1248  CA  SER A 160      63.167  28.394  14.076  1.00 28.89      A
ATOM   1249  CB  SER A 160      63.885  28.551  12.734  1.00 27.34      A
ATOM   1250  OG  SER A 160      65.206  28.053  12.807  1.00 29.49      A
ATOM   1251  C   SER A 160      63.241  26.957  14.565  1.00 27.42      A
ATOM   1252  O   SER A 160      64.092  26.628  15.392  1.00 25.45      A
ATOM   1253  N   TYR A 161      62.359  26.101  14.066  1.00 24.73      A
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ATOM   1254  CA  TYR A 161      62.359  24.725  14.517  1.00 24.26      A
ATOM   1255  CB  TYR A 161      61.172  24.480  15.451  1.00 23.50      A
ATOM   1256  CG  TYR A 161      60.935  25.593  16.434  1.00 24.01      A
ATOM   1257  CD1 TYR A 161      60.255  26.748  16.052  1.00 26.02      A
ATOM   1258  CE1 TYR A 161      60.009  27.774  16.959  1.00 27.93      A
ATOM   1259  CD2 TYR A 161      61.374  25.491  17.753  1.00 24.78      A
ATOM   1260  CE2 TYR A 161      61.136  26.514  18.674  1.00 25.93      A
ATOM   1261  CZ  TYR A 161      60.450  27.650  18.270  1.00 27.56      A
ATOM   1262  OH  TYR A 161      60.182  28.650  19.173  1.00 29.78      A
ATOM   1263  C   TYR A 161      62.330  23.700  13.397  1.00 25.15      A
ATOM   1264  O   TYR A 161      62.082  24.021  12.239  1.00 24.96      A
ATOM   1265  N   ASP A 162      62.600  22.455  13.775  1.00 26.26      A
ATOM   1266  CA  ASP A 162      62.598  21.331  12.858  1.00 26.94      A
ATOM   1267  CB  ASP A 162      64.007  21.014  12.356  1.00 30.11      A
ATOM   1268  CG  ASP A 162      64.548  22.067  11.434  1.00 32.85      A
ATOM   1269  OD1 ASP A 162      64.075  22.138  10.277  1.00 33.31      A
ATOM   1270  OD2 ASP A 162      65.443  22.819  11.874  1.00 33.08      A
ATOM   1271  C   ASP A 162      62.122  20.117  13.613  1.00 25.87      A
ATOM   1272  O   ASP A 162      62.449  19.947  14.789  1.00 24.38      A
ATOM   1273  N   CYS A 163      61.352  19.277  12.935  1.00 23.95      A
ATOM   1274  CA  CYS A 163      60.914  18.027  13.530  1.00 24.46      A
ATOM   1275  C   CYS A 163      61.916  17.043  12.938  1.00 22.46      A
ATOM   1276  O   CYS A 163      62.110  17.021  11.726  1.00 24.01      A
ATOM   1277  CB  CYS A 163      59.497  17.658  13.083  1.00 24.14      A
ATOM   1278  SG  CYS A 163      58.931  16.101  13.836  1.00 30.35      A
ATOM   1279  N   LYS A 164      62.571  16.259  13.782  1.00 22.96      A
ATOM   1280  CA  LYS A 164      63.559  15.292  13.307  1.00 24.69      A
ATOM   1281  CB  LYS A 164      64.867  15.450  14.089  1.00 27.54      A
ATOM   1282  CG  LYS A 164      65.977  14.490  13.689  1.00 28.93      A
ATOM   1283  CD  LYS A 164      67.179  14.643  14.622  1.00 32.03      A
ATOM   1284  CE  LYS A 164      68.254  13.596  14.350  1.00 33.85      A
ATOM   1285  NZ  LYS A 164      69.319  13.607  15.398  1.00 36.46      A
ATOM   1286  C   LYS A 164      63.023  13.875  13.463  1.00 24.25      A
ATOM   1287  O   LYS A 164      62.697  13.443  14.570  1.00 23.52      A
ATOM   1288  N   VAL A 165      62.931  13.160  12.345  1.00 23.37      A
ATOM   1289  CA  VAL A 165      62.415  11.797  12.344  1.00 24.06      A
ATOM   1290  CB  VAL A 165      61.174  11.682  11.408  1.00 23.45      A
ATOM   1291  CG1 VAL A 165      60.657  10.248  11.382  1.00 18.80      A
ATOM   1292  CG2 VAL A 165      60.078  12.632  11.878  1.00 22.37      A
ATOM   1293  C   VAL A 165      63.457  10.772  11.903  1.00 25.04      A
ATOM   1294  O   VAL A 165      64.103  10.931  10.869  1.00 25.12      A
ATOM   1295  N   GLU A 166      63.621   9.725  12.703  1.00 26.91      A
ATOM   1296  CA  GLU A 166      64.556   8.648  12.383  1.00 28.84      A
ATOM   1297  CB  GLU A 166      65.554   8.424  13.523  1.00 30.71      A
ATOM   1298  CG  GLU A 166      66.382   9.634  13.922  1.00 36.90      A
ATOM   1299  CD  GLU A 166      67.247   9.356  15.147  1.00 39.97      A
ATOM   1300  OE1 GLU A 166      67.466  10.286  15.954  1.00 43.02      A
ATOM   1301  OE2 GLU A 166      67.714   8.206  15.301  1.00 43.24      A
ATOM   1302  C   GLU A 166      63.739   7.369  12.183  1.00 28.96      A
ATOM   1303  O   GLU A 166      62.975   6.971  13.067  1.00 27.40      A
ATOM   1304  N   HIS A 167      63.910   6.728  11.029  1.00 29.87      A
ATOM   1305  CA  HIS A 167      63.189   5.496  10.713  1.00 30.70      A
ATOM   1306  CB  HIS A 167      61.838   5.833  10.084  1.00 30.90      A
ATOM   1307  CG  HIS A 167      60.932   4.655   9.933  1.00 34.01      A
ATOM   1308  CD2 HIS A 167      60.698   3.842   8.876  1.00 33.60      A
ATOM   1309  ND1 HIS A 167      60.159   4.172  10.967  1.00 36.69      A
ATOM   1310  CE1 HIS A 167      59.488   3.112  10.554  1.00 34.84      A
ATOM   1311  NE2 HIS A 167      59.798   2.890   9.290  1.00 34.90      A
ATOM   1312  C   HIS A 167      63.999   4.639   9.739  1.00 31.21      A
ATOM   1313  O   HIS A 167      64.696   5.167   8.866  1.00 29.44      A
ATOM   1314  N   TRP A 168      63.895   3.320   9.879  1.00 31.70      A
ATOM   1315  CA  TRP A 168      64.625   2.402   9.006  1.00 31.76      A
ATOM   1316  CB  TRP A 168      64.344   0.954   9.396  1.00 30.39      A
ATOM   1317  CG  TRP A 168      64.735   0.650  10.797  1.00 28.49      A
ATOM   1318  CD2 TRP A 168      64.115  -0.297  11.666  1.00 28.31      A
ATOM   1319  CE2 TRP A 168      64.837  -0.288  12.878  1.00 28.31      A
ATOM   1320  CE3 TRP A 168      63.017  -1.157  11.538  1.00 26.47      A
ATOM   1321  CD1 TRP A 168      65.778   1.184  11.491  1.00 28.32      A
ATOM   1322  NE1 TRP A 168      65.849   0.627  12.744  1.00 28.98      A
ATOM   1323  CZ2 TRP A 168      64.498  -1.107  13.958  1.00 28.85      A
ATOM   1324  CZ3 TRP A 168      62.678  -1.970  12.608  1.00 27.57      A
ATOM   1325  CH2 TRP A 168      63.418  -1.940  13.805  1.00 29.20      A
ATOM   1326  C   TRP A 168      64.332   2.588   7.523  1.00 33.06      A
ATOM   1327  O   TRP A 168      65.190   2.314   6.682  1.00 32.28      A
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| ATOM | 1328 | N | GLY A 169 | 63.126 | 3.049 | 7.202 | 1.00 34.81 | A |
|------|------|------|-----------|--------|--------|--------|------------|---|
| ATOM | 1329 | CA | GLY A 169 | 62.760 | 3.263 | 5.810 | 1.00 35.23 | A |
| ATOM | 1330 | C | GLY A 169 | 63.267 | 4.588 | 5.266 | 1.00 37.25 | A |
| ATOM | 1331 | O | GLY A 169 | 62.907 | 4.992 | 4.162 | 1.00 37.65 | A |
| ATOM | 1332 | N | LEU A 170 | 64.100 | 5.268 | 6.049 | 1.00 39.27 | A |
| ATOM | 1333 | CA | LEU A 170 | 64.673 | 6.555 | 5.660 | 1.00 41.10 | A |
| ATOM | 1334 | CB | LEU A 170 | 64.354 | 7.626 | 6.706 | 1.00 38.47 | A |
| ATOM | 1335 | CG | LEU A 170 | 62.923 | 8.143 | 6.843 | 1.00 38.66 | A |
| ATOM | 1336 | CD1 | LEU A 170 | 62.790 | 8.919 | 8.142 | 1.00 37.48 | A |
| ATOM | 1337 | CD2 | LEU A 170 | 62.572 | 9.017 | 5.653 | 1.00 37.65 | A |
| ATOM | 1338 | C | LEU A 170 | 66.183 | 6.425 | 5.556 | 1.00 43.62 | A |
| ATOM | 1339 | O | LEU A 170 | 66.809 | 5.762 | 6.382 | 1.00 44.45 | A |
| ATOM | 1340 | N | ASP A 171 | 66.764 | 7.066 | 4.545 | 1.00 46.98 | A |
| ATOM | 1341 | CA | ASP A 171 | 68.211 | 7.036 | 4.350 | 1.00 48.99 | A |
| ATOM | 1342 | CB | ASP A 171 | 68.602 | 7.810 | 3.086 | 1.00 51.12 | A |
| ATOM | 1343 | CG | ASP A 171 | 67.735 | 7.466 | 1.895 | 1.00 53.30 | A |
| ATOM | 1344 | OD1 | ASP A 171 | 66.520 | 7.761 | 1.936 | 1.00 54.82 | A |
| ATOM | 1345 | OD2 | ASP A 171 | 68.271 | 6.903 | 0.917 | 1.00 54.86 | A |
| ATOM | 1346 | C | ASP A 171 | 68.836 | 7.726 | 5.554 | 1.00 48.82 | A |
| ATOM | 1347 | O | ASP A 171 | 69.437 | 7.093 | 6.420 | 1.00 48.88 | A |
| ATOM | 1348 | N | LYS A 172 | 68.673 | 9.044 | 5.585 | 1.00 48.96 | A |
| ATOM | 1349 | CA | LYS A 172 | 69.192 | 9.877 | 6.659 | 1.00 48.79 | A |
| ATOM | 1350 | CB | LYS A 172 | 69.986 | 11.059 | 6.084 | 1.00 51.32 | A |
| ATOM | 1351 | CG | LYS A 172 | 71.074 | 10.698 | 5.075 | 1.00 55.53 | A |
| ATOM | 1352 | CD | LYS A 172 | 71.799 | 11.952 | 4.571 | 1.00 57.81 | A |
| ATOM | 1353 | CE | LYS A 172 | 72.859 | 11.621 | 3.518 | 1.00 59.22 | A |
| ATOM | 1354 | NZ | LYS A 172 | 73.912 | 10.702 | 4.038 | 1.00 58.32 | A |
| ATOM | 1355 | C | LYS A 172 | 67.990 | 10.419 | 7.420 | 1.00 46.36 | A |
| ATOM | 1356 | O | LYS A 172 | 66.862 | 10.381 | 6.919 | 1.00 44.39 | A |
| ATOM | 1357 | N | PRO A 173 | 68.211 | 10.920 | 8.645 | 1.00 44.20 | A |
| ATOM | 1358 | CD | PRO A 173 | 69.432 | 10.866 | 9.469 | 1.00 44.15 | A |
| ATOM | 1359 | CA | PRO A 173 | 67.089 | 11.462 | 9.410 | 1.00 42.74 | A |
| ATOM | 1360 | CB | PRO A 173 | 67.768 | 12.050 | 10.637 | 1.00 42.02 | A |
| ATOM | 1361 | CG | PRO A 173 | 68.887 | 11.080 | 10.872 | 1.00 44.25 | A |
| ATOM | 1362 | C | PRO A 173 | 66.369 | 12.517 | 8.578 | 1.00 41.09 | A |
| ATOM | 1363 | O | PRO A 173 | 67.002 | 13.309 | 7.877 | 1.00 39.67 | A |
| ATOM | 1364 | N | LEU A 174 | 65.044 | 12.502 | 8.636 | 1.00 39.80 | A |
| ATOM | 1365 | CA | LEU A 174 | 64.241 | 13.457 | 7.888 | 1.00 38.58 | A |
| ATOM | 1366 | CB | LEU A 174 | 62.894 | 12.838 | 7.522 | 1.00 38.73 | A |
| ATOM | 1367 | CG | LEU A 174 | 62.202 | 13.329 | 6.251 | 1.00 39.18 | A |
| ATOM | 1368 | CD1 | LEU A 174 | 60.826 | 12.691 | 6.170 | 1.00 39.20 | A |
| ATOM | 1369 | CD2 | LEU A 174 | 62.093 | 14.836 | 6.245 | 1.00 40.87 | A |
| ATOM | 1370 | C | LEU A 174 | 64.019 | 14.662 | 8.785 | 1.00 37.43 | A |
| ATOM | 1371 | O | LEU A 174 | 63.630 | 14.514 | 9.943 | 1.00 37.68 | A |
| ATOM | 1372 | N | LEU A 175 | 64.284 | 15.849 | 8.255 | 1.00 35.85 | A |
| ATOM | 1373 | CA | LEU A 175 | 64.098 | 17.077 | 9.012 | 1.00 34.38 | A |
| ATOM | 1374 | CB | LEU A 175 | 65.400 | 17.882 | 9.074 | 1.00 33.21 | A |
| ATOM | 1375 | CG | LEU A 175 | 66.425 | 17.502 | 10.147 | 1.00 34.82 | A |
| ATOM | 1376 | CD1 | LEU A 175 | 65.838 | 17.768 | 11.526 | 1.00 34.32 | A |
| ATOM | 1377 | CD2 | LEU A 175 | 66.819 | 16.038 | 10.008 | 1.00 35.37 | A |
| ATOM | 1378 | C | LEU A 175 | 63.020 | 17.898 | 8.337 | 1.00 33.09 | A |
| ATOM | 1379 | O | LEU A 175 | 63.080 | 18.137 | 7.132 | 1.00 33.84 | A |
| ATOM | 1380 | N | LYS A 176 | 62.023 | 18.312 | 9.108 | 1.00 30.14 | A |
| ATOM | 1381 | CA | LYS A 176 | 60.943 | 19.119 | 8.566 | 1.00 30.03 | A |
| ATOM | 1382 | CB | LYS A 176 | 59.598 | 18.416 | 8.772 | 1.00 30.60 | A |
| ATOM | 1383 | CG | LYS A 176 | 58.463 | 19.049 | 8.010 | 1.00 33.60 | A |
| ATOM | 1384 | CD | LYS A 176 | 58.742 | 19.054 | 6.508 | 1.00 37.73 | A |
| ATOM | 1385 | CE | LYS A 176 | 58.869 | 17.642 | 5.960 | 1.00 37.37 | A |
| ATOM | 1386 | NZ | LYS A 176 | 59.075 | 17.629 | 4.484 | 1.00 41.15 | A |
| ATOM | 1387 | C | LYS A 176 | 60.976 | 20.457 | 9.292 | 1.00 28.62 | A |
| ATOM | 1388 | O | LYS A 176 | 60.764 | 20.524 | 10.501 | 1.00 27.68 | A |
| ATOM | 1389 | N | HIS A 177 | 61.238 | 21.520 | 8.539 | 1.00 28.72 | A |
| ATOM | 1390 | CA | HIS A 177 | 61.353 | 22.868 | 9.088 | 1.00 29.54 | A |
| ATOM | 1391 | CB | HIS A 177 | 62.284 | 23.691 | 8.195 | 1.00 29.51 | A |
| ATOM | 1392 | CG | HIS A 177 | 62.485 | 25.097 | 8.663 | 1.00 30.53 | A |
| ATOM | 1393 | CD2 | HIS A 177 | 62.124 | 26.282 | 8.114 | 1.00 31.99 | A |
| ATOM | 1394 | ND1 | HIS A 177 | 63.117 | 25.401 | 9.849 | 1.00 32.09 | A |
| ATOM | 1395 | CE1 | HIS A 177 | 63.138 | 26.713 | 10.010 | 1.00 32.65 | A |
| ATOM | 1396 | NE2 | HIS A 177 | 62.542 | 27.271 | 8.971 | 1.00 32.04 | A |
| ATOM | 1397 | C | HIS A 177 | 60.059 | 23.654 | 9.304 | 1.00 29.24 | A |
| ATOM | 1398 | O | HIS A 177 | 59.100 | 23.519 | 8.549 | 1.00 27.66 | A |
| ATOM | 1399 | N | TRP A 178 | 60.062 | 24.492 | 10.340 | 1.00 30.09 | A |
| ATOM | 1400 | CA | TRP A 178 | 58.926 | 25.350 | 10.674 | 1.00 33.43 | A |
| ATOM | 1401 | CB | TRP A 178 | 57.959 | 24.647 | 11.632 | 1.00 28.07 | A |

| ATOM | 1402 | CG | TRP | A | 178 | 56.681 | 25.422 | 11.851 | 1.00 | 25.25 | A |
|------|------|------|------|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1403 | CD2 | TRP | A | 178 | 56.476 | 26.518 | 12.761 | 1.00 | 21.68 | A |
| ATOM | 1404 | CE2 | TRP | A | 178 | 55.138 | 26.942 | 12.611 | 1.00 | 20.86 | A |
| ATOM | 1405 | CE3 | TRP | A | 178 | 57.292 | 27.178 | 13.688 | 1.00 | 20.72 | A |
| ATOM | 1406 | CD1 | TRP | A | 178 | 55.489 | 25.239 | 11.206 | 1.00 | 24.81 | A |
| ATOM | 1407 | NE1 | TRP | A | 178 | 54.559 | 26.146 | 11.657 | 1.00 | 21.51 | A |
| ATOM | 1408 | CZ2 | TRP | A | 178 | 54.598 | 27.999 | 13.354 | 1.00 | 21.11 | A |
| ATOM | 1409 | CZ3 | TRP | A | 178 | 56.754 | 28.229 | 14.428 | 1.00 | 21.58 | A |
| ATOM | 1410 | CH2 | TRP | A | 178 | 55.419 | 28.627 | 14.255 | 1.00 | 20.94 | A |
| ATOM | 1411 | C | TRP | A | 178 | 59.425 | 26.628 | 11.348 | 1.00 | 36.30 | A |
| ATOM | 1412 | O | TRP | A | 178 | 60.314 | 26.591 | 12.195 | 1.00 | 36.91 | A |
| ATOM | 1413 | N | GLU | A | 179 | 58.852 | 27.761 | 10.975 | 1.00 | 40.65 | A |
| ATOM | 1414 | CA | GLU | A | 179 | 59.240 | 29.029 | 11.587 | 1.00 | 45.62 | A |
| ATOM | 1415 | CB | GLU | A | 179 | 60.481 | 29.622 | 10.899 | 1.00 | 47.42 | A |
| ATOM | 1416 | CG | GLU | A | 179 | 60.323 | 29.868 | 9.404 | 1.00 | 52.77 | A |
| ATOM | 1417 | CD | GLU | A | 179 | 61.498 | 30.624 | 8.806 | 1.00 | 55.17 | A |
| ATOM | 1418 | OE1 | GLU | A | 179 | 62.653 | 30.179 | 8.987 | 1.00 | 57.20 | A |
| ATOM | 1419 | OE2 | GLU | A | 179 | 61.265 | 31.663 | 8.149 | 1.00 | 57.21 | A |
| ATOM | 1420 | C | GLU | A | 179 | 58.074 | 30.001 | 11.489 | 1.00 | 46.47 | A |
| ATOM | 1421 | O | GLU | A | 179 | 57.322 | 29.983 | 10.513 | 1.00 | 45.49 | A |
| ATOM | 1422 | N | PRO | A | 180 | 57.898 | 30.855 | 12.509 | 1.00 | 47.97 | A |
| ATOM | 1423 | CD | PRO | A | 180 | 58.679 | 31.008 | 13.752 | 1.00 | 48.35 | A |
| ATOM | 1424 | CA | PRO | A | 180 | 56.789 | 31.810 | 12.460 | 1.00 | 49.45 | A |
| ATOM | 1425 | CB | PRO | A | 180 | 56.763 | 32.372 | 13.880 | 1.00 | 49.39 | A |
| ATOM | 1426 | CG | PRO | A | 180 | 58.214 | 32.358 | 14.266 | 1.00 | 48.65 | A |
| ATOM | 1427 | C | PRO | A | 180 | 57.014 | 32.891 | 11.401 | 1.00 | 50.21 | A |
| ATOM | 1428 | O | PRO | A | 180 | 58.174 | 33.041 | 10.950 | 1.00 | 49.95 | A |
| ATOM | 1429 | OXT | PRO | A | 180 | 56.030 | 33.578 | 11.043 | 1.00 | 50.90 | A |
| ATOM | 1430 | CB | SER | B | 3 | 67.953 | -2.426 | 7.203 | 1.00 | 59.72 | B |
| ATOM | 1431 | OG | SER | B | 3 | 68.517 | -3.384 | 6.321 | 1.00 | 60.71 | B |
| ATOM | 1432 | C | SER | B | 3 | 68.164 | -3.822 | 9.277 | 1.00 | 57.49 | B |
| ATOM | 1433 | O | SER | B | 3 | 68.117 | -4.879 | 8.642 | 1.00 | 57.32 | B |
| ATOM | 1434 | N | SER | B | 3 | 70.072 | -2.418 | 8.486 | 1.00 | 59.35 | B |
| ATOM | 1435 | CA | SER | B | 3 | 68.586 | -2.517 | 8.597 | 1.00 | 58.84 | B |
| ATOM | 1436 | N | PRO | B | 4 | 67.855 | -3.763 | 10.585 | 1.00 | 55.71 | B |
| ATOM | 1437 | CD | PRO | B | 4 | 67.914 | -2.580 | 11.463 | 1.00 | 54.97 | B |
| ATOM | 1438 | CA | PRO | B | 4 | 67.438 | -4.952 | 11.338 | 1.00 | 53.72 | B |
| ATOM | 1439 | CB | PRO | B | 4 | 67.457 | -4.467 | 12.787 | 1.00 | 54.71 | B |
| ATOM | 1440 | CG | PRO | B | 4 | 67.095 | -3.021 | 12.660 | 1.00 | 54.93 | B |
| ATOM | 1441 | C | PRO | B | 4 | 66.069 | -5.487 | 10.918 | 1.00 | 51.05 | B |
| ATOM | 1442 | O | PRO | B | 4 | 65.240 | -4.753 | 10.379 | 1.00 | 50.96 | B |
| ATOM | 1443 | N | GLU | B | 5 | 65.843 | -6.773 | 11.165 | 1.00 | 47.90 | B |
| ATOM | 1444 | CA | GLU | B | 5 | 64.581 | -7.410 | 10.810 | 1.00 | 45.24 | B |
| ATOM | 1445 | CB | GLU | B | 5 | 64.811 | -8.893 | 10.489 | 1.00 | 48.23 | B |
| ATOM | 1446 | CG | GLU | B | 5 | 65.603 | -9.656 | 11.545 | 1.00 | 54.54 | B |
| ATOM | 1447 | CD | GLU | B | 5 | 65.896 | -11.102 | 11.140 | 1.00 | 57.83 | B |
| ATOM | 1448 | OE1 | GLU | B | 5 | 66.421 | -11.317 | 10.024 | 1.00 | 59.67 | B |
| ATOM | 1449 | OE2 | GLU | B | 5 | 65.609 | -12.020 | 11.941 | 1.00 | 59.33 | B |
| ATOM | 1450 | C | GLU | B | 5 | 63.548 | -7.269 | 11.920 | 1.00 | 40.85 | B |
| ATOM | 1451 | O | GLU | B | 5 | 63.876 | -7.328 | 13.105 | 1.00 | 40.81 | B |
| ATOM | 1452 | N | ASP | B | 6 | 62.294 | -7.083 | 11.532 | 1.00 | 36.03 | B |
| ATOM | 1453 | CA | ASP | B | 6 | 61.223 | -6.936 | 12.508 | 1.00 | 32.11 | B |
| ATOM | 1454 | CB | ASP | B | 6 | 60.833 | -5.460 | 12.616 | 1.00 | 29.96 | B |
| ATOM | 1455 | CG | ASP | B | 6 | 59.933 | -5.171 | 13.798 | 1.00 | 27.91 | B |
| ATOM | 1456 | OD1 | ASP | B | 6 | 59.280 | -4.110 | 13.785 | 1.00 | 29.62 | B |
| ATOM | 1457 | OD2 | ASP | B | 6 | 59.884 | -5.982 | 14.745 | 1.00 | 29.86 | B |
| ATOM | 1458 | C | ASP | B | 6 | 60.014 | -7.766 | 12.077 | 1.00 | 29.68 | B |
| ATOM | 1459 | O | ASP | B | 6 | 59.676 | -7.802 | 10.899 | 1.00 | 29.14 | B |
| ATOM | 1460 | N | PHE | B | 7 | 59.380 | -8.438 | 13.032 | 1.00 | 27.77 | B |
| ATOM | 1461 | CA | PHE | B | 7 | 58.193 | -9.249 | 12.765 | 1.00 | 28.11 | B |
| ATOM | 1462 | CB | PHE | B | 7 | 58.453 | -10.704 | 13.161 | 1.00 | 29.55 | B |
| ATOM | 1463 | CG | PHE | B | 7 | 59.461 | -11.385 | 12.282 | 1.00 | 31.06 | B |
| ATOM | 1464 | CD1 | PHE | B | 7 | 59.126 | -11.766 | 10.989 | 1.00 | 29.85 | B |
| ATOM | 1465 | CD2 | PHE | B | 7 | 60.761 | -11.603 | 12.730 | 1.00 | 32.21 | B |
| ATOM | 1466 | CE1 | PHE | B | 7 | 60.073 | -12.355 | 10.145 | 1.00 | 33.75 | B |
| ATOM | 1467 | CE2 | PHE | B | 7 | 61.719 | -12.190 | 11.897 | 1.00 | 34.27 | B |
| ATOM | 1468 | CZ | PHE | B | 7 | 61.373 | -12.568 | 10.599 | 1.00 | 33.07 | B |
| ATOM | 1469 | C | PHE | B | 7 | 57.032 | -8.657 | 13.562 | 1.00 | 26.58 | B |
| ATOM | 1470 | O | PHE | B | 7 | 57.046 | -8.645 | 14.794 | 1.00 | 25.72 | B |
| ATOM | 1471 | N | VAL | B | 8 | 56.023 | -8.174 | 12.849 | 1.00 | 25.17 | B |
| ATOM | 1472 | CA | VAL | B | 8 | 54.891 | -7.520 | 13.493 | 1.00 | 23.46 | B |
| ATOM | 1473 | CB | VAL | B | 8 | 54.670 | -6.132 | 12.871 | 1.00 | 21.55 | B |
| ATOM | 1474 | CG1 | VAL | B | 8 | 53.573 | -5.394 | 13.612 | 1.00 | 21.83 | B |
| ATOM | 1475 | CG2 | VAL | B | 8 | 55.975 | -5.342 | 12.895 | 1.00 | 21.30 | B |

| ATOM | 1476 | C   | VAL | B | 8  | 53.556 | -8.255  | 13.467 | 1.00 | 24.08 | B |
| ---- | ---- | --- | --- | - | -- | ------ | ------- | ------ | ---- | ----- | - |
| ATOM | 1477 | O   | VAL | B | 8  | 53.204 | -8.912  | 12.491 | 1.00 | 23.46 | B |
| ATOM | 1478 | N   | TYR | B | 9  | 52.804 | -8.127  | 14.554 | 1.00 | 23.26 | B |
| ATOM | 1479 | CA  | TYR | B | 9  | 51.493 | -8.747  | 14.619 | 1.00 | 23.18 | B |
| ATOM | 1480 | CB  | TYR | B | 9  | 51.510 | -9.978  | 15.520 | 1.00 | 23.12 | B |
| ATOM | 1481 | CG  | TYR | B | 9  | 50.231 | -10.786 | 15.465 | 1.00 | 24.54 | B |
| ATOM | 1482 | CD1 | TYR | B | 9  | 50.158 | -11.962 | 14.722 | 1.00 | 26.50 | B |
| ATOM | 1483 | CE1 | TYR | B | 9  | 49.000 | -12.743 | 14.716 | 1.00 | 25.08 | B |
| ATOM | 1484 | CD2 | TYR | B | 9  | 49.108 | -10.399 | 16.190 | 1.00 | 22.88 | B |
| ATOM | 1485 | CE2 | TYR | B | 9  | 47.948 | -11.165 | 16.188 | 1.00 | 23.91 | B |
| ATOM | 1486 | CZ  | TYR | B | 9  | 47.902 | -12.342 | 15.455 | 1.00 | 24.87 | B |
| ATOM | 1487 | OH  | TYR | B | 9  | 46.780 | -13.140 | 15.501 | 1.00 | 25.45 | B |
| ATOM | 1488 | C   | TYR | B | 9  | 50.509 | -7.723  | 15.163 | 1.00 | 21.33 | B |
| ATOM | 1489 | O   | TYR | B | 9  | 50.798 | -7.028  | 16.133 | 1.00 | 22.92 | B |
| ATOM | 1490 | N   | GLN | B | 10 | 49.353 | -7.622  | 14.521 | 1.00 | 19.98 | B |
| ATOM | 1491 | CA  | GLN | B | 10 | 48.326 | -6.687  | 14.952 | 1.00 | 19.52 | B |
| ATOM | 1492 | CB  | GLN | B | 10 | 48.171 | -5.523  | 13.962 | 1.00 | 19.13 | B |
| ATOM | 1493 | CG  | GLN | B | 10 | 49.433 | -4.810  | 13.509 | 1.00 | 19.33 | B |
| ATOM | 1494 | CD  | GLN | B | 10 | 49.117 | -3.708  | 12.499 | 1.00 | 17.96 | B |
| ATOM | 1495 | OE1 | GLN | B | 10 | 48.336 | -2.802  | 12.783 | 1.00 | 18.49 | B |
| ATOM | 1496 | NE2 | GLN | B | 10 | 49.715 | -3.790  | 11.316 | 1.00 | 19.41 | B |
| ATOM | 1497 | C   | GLN | B | 10 | 46.967 | -7.375  | 15.029 | 1.00 | 19.74 | B |
| ATOM | 1498 | O   | GLN | B | 10 | 46.626 | -8.227  | 14.192 | 1.00 | 18.98 | B |
| ATOM | 1499 | N   | PHE | B | 11 | 46.195 | -6.996  | 16.040 | 1.00 | 19.06 | B |
| ATOM | 1500 | CA  | PHE | B | 11 | 44.842 | -7.487  | 16.182 | 1.00 | 16.54 | B |
| ATOM | 1501 | CB  | PHE | B | 11 | 44.668 | -8.454  | 17.336 | 1.00 | 17.48 | B |
| ATOM | 1502 | CG  | PHE | B | 11 | 43.237 | -8.847  | 17.544 | 1.00 | 16.17 | B |
| ATOM | 1503 | CD1 | PHE | B | 11 | 42.570 | -9.604  | 16.582 | 1.00 | 17.49 | B |
| ATOM | 1504 | CD2 | PHE | B | 11 | 42.536 | -8.406  | 18.656 | 1.00 | 14.41 | B |
| ATOM | 1505 | CE1 | PHE | B | 11 | 41.219 | -9.913  | 16.725 | 1.00 | 18.03 | B |
| ATOM | 1506 | CE2 | PHE | B | 11 | 41.191 | -8.708  | 18.814 | 1.00 | 16.34 | B |
| ATOM | 1507 | CZ  | PHE | B | 11 | 40.528 | -9.463  | 17.845 | 1.00 | 17.60 | B |
| ATOM | 1508 | C   | PHE | B | 11 | 43.984 | -6.271  | 16.450 | 1.00 | 18.14 | B |
| ATOM | 1509 | O   | PHE | B | 11 | 44.241 | -5.506  | 17.386 | 1.00 | 15.63 | B |
| ATOM | 1510 | N   | LYS | B | 12 | 42.961 | -6.094  | 15.625 | 1.00 | 17.33 | B |
| ATOM | 1511 | CA  | LYS | B | 12 | 42.082 | -4.958  | 15.770 | 1.00 | 17.63 | B |
| ATOM | 1512 | CB  | LYS | B | 12 | 42.188 | -4.067  | 14.536 | 1.00 | 18.71 | B |
| ATOM | 1513 | CG  | LYS | B | 12 | 43.599 | -3.642  | 14.192 | 1.00 | 15.90 | B |
| ATOM | 1514 | CD  | LYS | B | 12 | 43.602 | -2.909  | 12.871 | 1.00 | 17.33 | B |
| ATOM | 1515 | CE  | LYS | B | 12 | 44.946 | -2.297  | 12.570 | 1.00 | 18.72 | B |
| ATOM | 1516 | NZ  | LYS | B | 12 | 44.838 | -1.450  | 11.340 | 1.00 | 20.93 | B |
| ATOM | 1517 | C   | LYS | B | 12 | 40.632 | -5.387  | 15.968 | 1.00 | 18.92 | B |
| ATOM | 1518 | O   | LYS | B | 12 | 40.041 | -6.050  | 15.109 | 1.00 | 17.25 | B |
| ATOM | 1519 | N   | GLY | B | 13 | 40.076 | -5.002  | 17.114 | 1.00 | 17.59 | B |
| ATOM | 1520 | CA  | GLY | B | 13 | 38.701 | -5.322  | 17.430 | 1.00 | 19.88 | B |
| ATOM | 1521 | C   | GLY | B | 13 | 37.874 | -4.113  | 17.064 | 1.00 | 20.12 | B |
| ATOM | 1522 | O   | GLY | B | 13 | 37.515 | -3.309  | 17.923 | 1.00 | 21.08 | B |
| ATOM | 1523 | N   | MET | B | 14 | 37.561 | -4.000  | 15.779 | 1.00 | 20.42 | B |
| ATOM | 1524 | CA  | MET | B | 14 | 36.817 | -2.866  | 15.262 | 1.00 | 22.96 | B |
| ATOM | 1525 | CB  | MET | B | 14 | 37.334 | -2.554  | 13.866 | 1.00 | 23.02 | B |
| ATOM | 1526 | CG  | MET | B | 14 | 38.846 | -2.485  | 13.820 | 1.00 | 23.58 | B |
| ATOM | 1527 | SD  | MET | B | 14 | 39.449 | -2.095  | 12.191 | 1.00 | 26.23 | B |
| ATOM | 1528 | CE  | MET | B | 14 | 39.260 | -0.318  | 12.182 | 1.00 | 25.78 | B |
| ATOM | 1529 | C   | MET | B | 14 | 35.295 | -2.997  | 15.242 | 1.00 | 23.12 | B |
| ATOM | 1530 | O   | MET | B | 14 | 34.751 | -4.089  | 15.081 | 1.00 | 24.36 | B |
| ATOM | 1531 | N   | CYS | B | 15 | 34.628 | -1.860  | 15.427 | 1.00 | 24.04 | B |
| ATOM | 1532 | CA  | CYS | B | 15 | 33.173 | -1.768  | 15.433 | 1.00 | 24.91 | B |
| ATOM | 1533 | C   | CYS | B | 15 | 32.808 | -0.587  | 14.547 | 1.00 | 25.49 | B |
| ATOM | 1534 | O   | CYS | B | 15 | 33.369 | 0.504   | 14.700 | 1.00 | 23.97 | B |
| ATOM | 1535 | CB  | CYS | B | 15 | 32.630 | -1.489  | 16.847 | 1.00 | 26.02 | B |
| ATOM | 1536 | SG  | CYS | B | 15 | 32.691 | -2.831  | 18.084 | 1.00 | 33.69 | B |
| ATOM | 1537 | N   | TYR | B | 16 | 31.871 | -0.805  | 13.630 | 1.00 | 25.87 | B |
| ATOM | 1538 | CA  | TYR | B | 16 | 31.413 | 0.244   | 12.724 | 1.00 | 25.59 | B |
| ATOM | 1539 | CB  | TYR | B | 16 | 31.539 | -0.223  | 11.274 | 1.00 | 24.73 | B |
| ATOM | 1540 | CG  | TYR | B | 16 | 32.958 | -0.575  | 10.879 | 1.00 | 26.05 | B |
| ATOM | 1541 | CD1 | TYR | B | 16 | 33.523 | -1.795  | 11.239 | 1.00 | 22.96 | B |
| ATOM | 1542 | CE1 | TYR | B | 16 | 34.843 | -2.102  | 10.904 | 1.00 | 25.81 | B |
| ATOM | 1543 | CD2 | TYR | B | 16 | 33.748 | 0.334   | 10.171 | 1.00 | 25.30 | B |
| ATOM | 1544 | CE2 | TYR | B | 16 | 35.066 | 0.041   | 9.835  | 1.00 | 25.12 | B |
| ATOM | 1545 | CZ  | TYR | B | 16 | 35.607 | -1.176  | 10.202 | 1.00 | 26.66 | B |
| ATOM | 1546 | OH  | TYR | B | 16 | 36.908 | -1.463  | 9.868  | 1.00 | 29.22 | B |
| ATOM | 1547 | C   | TYR | B | 16 | 29.960 | 0.575   | 13.045 | 1.00 | 26.48 | B |
| ATOM | 1548 | O   | TYR | B | 16 | 29.113 | -0.315  | 13.091 | 1.00 | 26.41 | B |
| ATOM | 1549 | N   | PHE | B | 17 | 29.684 | 1.859   | 13.266 | 1.00 | 27.76 | B |

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| ATOM | 1550 | CA | PHE | B | 17 | 28.346 | 2.338 | 13.613 | 1.00 | 29.09 | B |
|------|------|------|------|------|------|------|------|------|------|------|------|
| ATOM | 1551 | CB | PHE | B | 17 | 28.382 | 3.047 | 14.967 | 1.00 | 28.08 | B |
| ATOM | 1552 | CG | PHE | B | 17 | 28.885 | 2.194 | 16.091 | 1.00 | 28.21 | B |
| ATOM | 1553 | CD1 | PHE | B | 17 | 28.056 | 1.253 | 16.693 | 1.00 | 27.20 | B |
| ATOM | 1554 | CD2 | PHE | B | 17 | 30.188 | 2.340 | 16.558 | 1.00 | 26.60 | B |
| ATOM | 1555 | CE1 | PHE | B | 17 | 28.519 | 0.470 | 17.752 | 1.00 | 28.13 | B |
| ATOM | 1556 | CE2 | PHE | B | 17 | 30.662 | 1.565 | 17.610 | 1.00 | 25.62 | B |
| ATOM | 1557 | CZ | PHE | B | 17 | 29.828 | 0.629 | 18.210 | 1.00 | 26.17 | B |
| ATOM | 1558 | C | PHE | B | 17 | 27.772 | 3.318 | 12.592 | 1.00 | 30.71 | B |
| ATOM | 1559 | O | PHE | B | 17 | 28.452 | 4.239 | 12.155 | 1.00 | 31.05 | B |
| ATOM | 1560 | N | THR | B | 18 | 26.506 | 3.125 | 12.237 | 1.00 | 33.51 | B |
| ATOM | 1561 | CA | THR | B | 18 | 25.831 | 4.005 | 11.291 | 1.00 | 36.95 | B |
| ATOM | 1562 | CB | THR | B | 18 | 25.797 | 3.395 | 9.875 | 1.00 | 37.23 | B |
| ATOM | 1563 | OG1 | THR | B | 18 | 27.133 | 3.105 | 9.447 | 1.00 | 40.77 | B |
| ATOM | 1564 | CG2 | THR | B | 18 | 25.171 | 4.369 | 8.891 | 1.00 | 38.43 | B |
| ATOM | 1565 | C | THR | B | 18 | 24.398 | 4.273 | 11.753 | 1.00 | 38.56 | B |
| ATOM | 1566 | O | THR | B | 18 | 23.671 | 3.351 | 12.131 | 1.00 | 38.36 | B |
| ATOM | 1567 | N | ASN | B | 19 | 24.007 | 5.544 | 11.726 | 1.00 | 39.80 | B |
| ATOM | 1568 | CA | ASN | B | 19 | 22.668 | 5.961 | 12.132 | 1.00 | 41.35 | B |
| ATOM | 1569 | CB | ASN | B | 19 | 21.638 | 5.465 | 11.110 | 1.00 | 41.21 | B |
| ATOM | 1570 | CG | ASN | B | 19 | 20.311 | 6.190 | 11.223 | 1.00 | 42.85 | B |
| ATOM | 1571 | OD1 | ASN | B | 19 | 20.271 | 7.378 | 11.548 | 1.00 | 42.24 | B |
| ATOM | 1572 | ND2 | ASN | B | 19 | 19.219 | 5.485 | 10.937 | 1.00 | 42.57 | B |
| ATOM | 1573 | C | ASN | B | 19 | 22.352 | 5.416 | 13.521 | 1.00 | 42.37 | B |
| ATOM | 1574 | O | ASN | B | 19 | 21.540 | 4.503 | 13.673 | 1.00 | 43.36 | B |
| ATOM | 1575 | N | GLY | B | 20 | 22.997 | 5.989 | 14.533 | 1.00 | 42.56 | B |
| ATOM | 1576 | CA | GLY | B | 20 | 22.790 | 5.535 | 15.894 | 1.00 | 43.89 | B |
| ATOM | 1577 | C | GLY | B | 20 | 23.293 | 4.110 | 16.031 | 1.00 | 45.10 | B |
| ATOM | 1578 | O | GLY | B | 20 | 24.421 | 3.807 | 15.646 | 1.00 | 44.28 | B |
| ATOM | 1579 | N | THR | B | 21 | 22.458 | 3.232 | 16.575 | 1.00 | 46.37 | B |
| ATOM | 1580 | CA | THR | B | 21 | 22.824 | 1.832 | 16.738 | 1.00 | 47.42 | B |
| ATOM | 1581 | CB | THR | B | 21 | 22.667 | 1.373 | 18.199 | 1.00 | 48.57 | B |
| ATOM | 1582 | OG1 | THR | B | 21 | 21.438 | 1.885 | 18.731 | 1.00 | 49.14 | B |
| ATOM | 1583 | CG2 | THR | B | 21 | 23.843 | 1.856 | 19.043 | 1.00 | 47.59 | B |
| ATOM | 1584 | C | THR | B | 21 | 21.958 | 0.947 | 15.846 | 1.00 | 48.74 | B |
| ATOM | 1585 | O | THR | B | 21 | 21.925 | -0.276 | 16.016 | 1.00 | 48.04 | B |
| ATOM | 1586 | N | GLU | B | 22 | 21.253 | 1.570 | 14.902 | 1.00 | 48.57 | B |
| ATOM | 1587 | CA | GLU | B | 22 | 20.405 | 0.822 | 13.979 | 1.00 | 48.90 | B |
| ATOM | 1588 | CB | GLU | B | 22 | 19.741 | 1.745 | 12.957 | 1.00 | 52.60 | B |
| ATOM | 1589 | CG | GLU | B | 22 | 18.669 | 2.667 | 13.493 | 1.00 | 58.06 | B |
| ATOM | 1590 | CD | GLU | B | 22 | 17.862 | 3.297 | 12.368 | 1.00 | 62.27 | B |
| ATOM | 1591 | OE1 | GLU | B | 22 | 17.027 | 4.185 | 12.648 | 1.00 | 63.99 | B |
| ATOM | 1592 | OE2 | GLU | B | 22 | 18.065 | 2.894 | 11.199 | 1.00 | 64.70 | B |
| ATOM | 1593 | C | GLU | B | 22 | 21.285 | -0.156 | 13.229 | 1.00 | 46.38 | B |
| ATOM | 1594 | O | GLU | B | 22 | 21.029 | -1.356 | 13.209 | 1.00 | 45.52 | B |
| ATOM | 1595 | N | ARG | B | 23 | 22.324 | 0.379 | 12.601 | 1.00 | 45.42 | B |
| ATOM | 1596 | CA | ARG | B | 23 | 23.260 | -0.438 | 11.844 | 1.00 | 44.59 | B |
| ATOM | 1597 | CB | ARG | B | 23 | 23.423 | 0.127 | 10.422 | 1.00 | 45.69 | B |
| ATOM | 1598 | CG | ARG | B | 23 | 22.169 | -0.062 | 9.554 | 1.00 | 49.95 | B |
| ATOM | 1599 | CD | ARG | B | 23 | 22.406 | 0.237 | 8.074 | 1.00 | 53.34 | B |
| ATOM | 1600 | NE | ARG | B | 23 | 22.153 | 1.632 | 7.708 | 1.00 | 55.57 | B |
| ATOM | 1601 | CZ | ARG | B | 23 | 20.949 | 2.200 | 7.700 | 1.00 | 57.20 | B |
| ATOM | 1602 | NH1 | ARG | B | 23 | 19.878 | 1.495 | 8.042 | 1.00 | 58.09 | B |
| ATOM | 1603 | NH2 | ARG | B | 23 | 20.813 | 3.471 | 7.340 | 1.00 | 56.82 | B |
| ATOM | 1604 | C | ARG | B | 23 | 24.606 | -0.534 | 12.567 | 1.00 | 40.56 | B |
| ATOM | 1605 | O | ARG | B | 23 | 25.306 | 0.459 | 12.748 | 1.00 | 41.15 | B |
| ATOM | 1606 | N | VAL | B | 24 | 24.944 | -1.743 | 12.995 | 1.00 | 38.17 | B |
| ATOM | 1607 | CA | VAL | B | 24 | 26.191 | -1.996 | 13.708 | 1.00 | 34.88 | B |
| ATOM | 1608 | CB | VAL | B | 24 | 25.931 | -2.314 | 15.200 | 1.00 | 34.41 | B |
| ATOM | 1609 | CG1 | VAL | B | 24 | 27.251 | -2.526 | 15.918 | 1.00 | 35.28 | B |
| ATOM | 1610 | CG2 | VAL | B | 24 | 25.146 | -1.190 | 15.852 | 1.00 | 34.70 | B |
| ATOM | 1611 | C | VAL | B | 24 | 26.909 | -3.194 | 13.100 | 1.00 | 32.34 | B |
| ATOM | 1612 | O | VAL | B | 24 | 26.287 | -4.214 | 12.812 | 1.00 | 33.23 | B |
| ATOM | 1613 | N | ARG | B | 25 | 28.217 | -3.076 | 12.898 | 1.00 | 30.18 | B |
| ATOM | 1614 | CA | ARG | B | 25 | 28.970 | -4.194 | 12.354 | 1.00 | 26.97 | B |
| ATOM | 1615 | CB | ARG | B | 25 | 29.225 | -4.022 | 10.852 | 1.00 | 27.67 | B |
| ATOM | 1616 | CG | ARG | B | 25 | 29.400 | -5.362 | 10.170 | 1.00 | 29.58 | B |
| ATOM | 1617 | CD | ARG | B | 25 | 30.406 | -5.363 | 9.052 | 1.00 | 31.26 | B |
| ATOM | 1618 | NE | ARG | B | 25 | 30.058 | -4.454 | 7.974 | 1.00 | 33.12 | B |
| ATOM | 1619 | CZ | ARG | B | 25 | 30.415 | -4.631 | 6.705 | 1.00 | 32.27 | B |
| ATOM | 1620 | NH1 | ARG | B | 25 | 31.124 | -5.695 | 6.346 | 1.00 | 31.13 | B |
| ATOM | 1621 | NH2 | ARG | B | 25 | 30.087 | -3.726 | 5.799 | 1.00 | 30.62 | B |
| ATOM | 1622 | C | ARG | B | 25 | 30.305 | -4.402 | 13.065 | 1.00 | 24.10 | B |
| ATOM | 1623 | O | ARG | B | 25 | 31.095 | -3.477 | 13.225 | 1.00 | 22.56 | B |

| ATOM | 1624 | N    | LEU B | 26 | 30.551 | -5.630  | 13.495 | 1.00 | 22.65 | B |
|------|------|------|-------|----|--------|---------|--------|------|-------|---|
| ATOM | 1625 | CA   | LEU B | 26 | 31.801 | -5.942  | 14.163 | 1.00 | 22.38 | B |
| ATOM | 1626 | CB   | LEU B | 26 | 31.558 | -6.888  | 15.345 | 1.00 | 20.25 | B |
| ATOM | 1627 | CG   | LEU B | 26 | 32.795 | -7.389  | 16.100 | 1.00 | 19.86 | B |
| ATOM | 1628 | CD1  | LEU B | 26 | 32.452 | -7.613  | 17.568 | 1.00 | 22.49 | B |
| ATOM | 1629 | CD2  | LEU B | 26 | 33.304 | -8.665  | 15.464 | 1.00 | 18.43 | B |
| ATOM | 1630 | C    | LEU B | 26 | 32.726 | -6.591  | 13.150 | 1.00 | 21.50 | B |
| ATOM | 1631 | O    | LEU B | 26 | 32.289 | -7.402  | 12.342 | 1.00 | 22.83 | B |
| ATOM | 1632 | N    | VAL B | 27 | 33.998 | -6.208  | 13.177 | 1.00 | 21.29 | B |
| ATOM | 1633 | CA   | VAL B | 27 | 34.984 | -6.780  | 12.270 | 1.00 | 20.66 | B |
| ATOM | 1634 | CB   | VAL B | 27 | 35.178 | -5.911  | 11.004 | 1.00 | 20.59 | B |
| ATOM | 1635 | CG1  | VAL B | 27 | 36.169 | -6.576  | 10.069 | 1.00 | 19.45 | B |
| ATOM | 1636 | CG2  | VAL B | 27 | 33.849 | -5.696  | 10.297 | 1.00 | 22.37 | B |
| ATOM | 1637 | C    | VAL B | 27 | 36.330 | -6.885  | 12.988 | 1.00 | 22.39 | B |
| ATOM | 1638 | O    | VAL B | 27 | 37.046 | -5.889  | 13.135 | 1.00 | 22.63 | B |
| ATOM | 1639 | N    | SER B | 28 | 36.673 | -8.083  | 13.450 | 1.00 | 21.32 | B |
| ATOM | 1640 | CA   | SER B | 28 | 37.947 | -8.259  | 14.130 | 1.00 | 21.51 | B |
| ATOM | 1641 | CB   | SER B | 28 | 37.831 | -9.284  | 15.275 | 1.00 | 19.72 | B |
| ATOM | 1642 | OG   | SER B | 28 | 37.542 | -10.581 | 14.819 | 1.00 | 24.33 | B |
| ATOM | 1643 | C    | SER B | 28 | 38.954 | -8.693  | 13.074 | 1.00 | 21.25 | B |
| ATOM | 1644 | O    | SER B | 28 | 38.661 | -9.537  | 12.229 | 1.00 | 19.44 | B |
| ATOM | 1645 | N    | ARG B | 29 | 40.137 | -8.089  | 13.106 | 1.00 | 20.61 | B |
| ATOM | 1646 | CA   | ARG B | 29 | 41.158 | -8.402  | 12.115 | 1.00 | 19.66 | B |
| ATOM | 1647 | CB   | ARG B | 29 | 41.418 | -7.169  | 11.230 | 1.00 | 19.91 | B |
| ATOM | 1648 | CG   | ARG B | 29 | 40.178 | -6.407  | 10.754 | 1.00 | 16.79 | B |
| ATOM | 1649 | CD   | ARG B | 29 | 40.608 | -5.121  | 10.031 | 1.00 | 18.10 | B |
| ATOM | 1650 | NE   | ARG B | 29 | 39.487 | -4.318  | 9.553  | 1.00 | 19.38 | B |
| ATOM | 1651 | CZ   | ARG B | 29 | 38.738 | -4.619  | 8.497  | 1.00 | 20.62 | B |
| ATOM | 1652 | NH1  | ARG B | 29 | 38.983 | -5.714  | 7.789  | 1.00 | 19.50 | B |
| ATOM | 1653 | NH2  | ARG B | 29 | 37.736 | -3.822  | 8.149  | 1.00 | 21.90 | B |
| ATOM | 1654 | C    | ARG B | 29 | 42.482 | -8.833  | 12.738 | 1.00 | 18.57 | B |
| ATOM | 1655 | O    | ARG B | 29 | 43.024 | -8.121  | 13.584 | 1.00 | 19.40 | B |
| ATOM | 1656 | N    | SER B | 30 | 42.991 | -9.995  | 12.326 | 1.00 | 18.99 | B |
| ATOM | 1657 | CA   | SER B | 30 | 44.284 | -10.501 | 12.797 | 1.00 | 21.66 | B |
| ATOM | 1658 | CB   | SER B | 30 | 44.241 | -12.015 | 13.023 | 1.00 | 22.77 | B |
| ATOM | 1659 | OG   | SER B | 30 | 43.390 | -12.352 | 14.106 | 1.00 | 26.81 | B |
| ATOM | 1660 | C    | SER B | 30 | 45.265 | -10.163 | 11.673 | 1.00 | 23.37 | B |
| ATOM | 1661 | O    | SER B | 30 | 45.055 | -10.553 | 10.522 | 1.00 | 21.31 | B |
| ATOM | 1662 | N    | ILE B | 31 | 46.338 | -9.450  | 12.009 | 1.00 | 24.76 | B |
| ATOM | 1663 | CA   | ILE B | 31 | 47.298 | -8.998  | 10.999 | 1.00 | 24.33 | B |
| ATOM | 1664 | CB   | ILE B | 31 | 47.341 | -7.440  | 10.958 | 1.00 | 25.20 | B |
| ATOM | 1665 | CG2  | ILE B | 31 | 47.982 | -6.964  | 9.672  | 1.00 | 23.24 | B |
| ATOM | 1666 | CG1  | ILE B | 31 | 45.934 | -6.857  | 11.106 | 1.00 | 26.96 | B |
| ATOM | 1667 | CD1  | ILE B | 31 | 45.032 | -7.136  | 9.947  | 1.00 | 31.25 | B |
| ATOM | 1668 | C    | ILE B | 31 | 48.741 | -9.460  | 11.187 | 1.00 | 23.98 | B |
| ATOM | 1669 | O    | ILE B | 31 | 49.298 | -9.318  | 12.272 | 1.00 | 22.29 | B |
| ATOM | 1670 | N    | TYR B | 32 | 49.345 | -9.993  | 10.123 | 1.00 | 25.50 | B |
| ATOM | 1671 | CA   | TYR B | 32 | 50.750 | -10.405 | 10.162 | 1.00 | 26.21 | B |
| ATOM | 1672 | CB   | TYR B | 32 | 50.965 | -11.764 | 9.492  | 1.00 | 28.46 | B |
| ATOM | 1673 | CG   | TYR B | 32 | 52.406 | -12.224 | 9.544  | 1.00 | 31.10 | B |
| ATOM | 1674 | CD1  | TYR B | 32 | 53.050 | -12.412 | 10.765 | 1.00 | 32.47 | B |
| ATOM | 1675 | CE1  | TYR B | 32 | 54.393 | -12.780 | 10.827 | 1.00 | 34.69 | B |
| ATOM | 1676 | CD2  | TYR B | 32 | 53.140 | -12.424 | 8.375  | 1.00 | 33.60 | B |
| ATOM | 1677 | CE2  | TYR B | 32 | 54.484 | -12.795 | 8.422  | 1.00 | 34.50 | B |
| ATOM | 1678 | CZ   | TYR B | 32 | 55.103 | -12.965 | 9.654  | 1.00 | 35.65 | B |
| ATOM | 1679 | OH   | TYR B | 32 | 56.438 | -13.281 | 9.717  | 1.00 | 37.73 | B |
| ATOM | 1680 | C    | TYR B | 32 | 51.478 | -9.307  | 9.384  | 1.00 | 25.67 | B |
| ATOM | 1681 | O    | TYR B | 32 | 51.273 | -9.140  | 8.174  | 1.00 | 24.75 | B |
| ATOM | 1682 | N    | ASN B | 33 | 52.319 | -8.559  | 10.094 | 1.00 | 25.63 | B |
| ATOM | 1683 | CA   | ASN B | 33 | 53.036 | -7.416  | 9.526  | 1.00 | 24.95 | B |
| ATOM | 1684 | CB   | ASN B | 33 | 53.955 | -7.848  | 8.379  | 1.00 | 23.75 | B |
| ATOM | 1685 | CG   | ASN B | 33 | 55.171 | -8.615  | 8.878  | 1.00 | 24.11 | B |
| ATOM | 1686 | OD1  | ASN B | 33 | 55.803 | -8.223  | 9.861  | 1.00 | 25.42 | B |
| ATOM | 1687 | ND2  | ASN B | 33 | 55.506 | -9.708  | 8.204  | 1.00 | 25.18 | B |
| ATOM | 1688 | C    | ASN B | 33 | 51.990 | -6.392  | 9.070  | 1.00 | 25.11 | B |
| ATOM | 1689 | O    | ASN B | 33 | 51.491 | -5.618  | 9.893  | 1.00 | 26.06 | B |
| ATOM | 1690 | N    | ARG B | 34 | 51.652 | -6.375  | 7.786  | 1.00 | 25.75 | B |
| ATOM | 1691 | CA   | ARG B | 34 | 50.631 | -5.449  | 7.296  | 1.00 | 27.64 | B |
| ATOM | 1692 | CB   | ARG B | 34 | 51.244 | -4.362  | 6.408  | 1.00 | 27.74 | B |
| ATOM | 1693 | CG   | ARG B | 34 | 51.972 | -3.257  | 7.158  | 1.00 | 29.94 | B |
| ATOM | 1694 | CD   | ARG B | 34 | 51.664 | -1.888  | 6.541  | 1.00 | 32.95 | B |
| ATOM | 1695 | NE   | ARG B | 34 | 51.897 | -1.875  | 5.101  | 1.00 | 35.17 | B |
| ATOM | 1696 | CZ   | ARG B | 34 | 51.392 | -0.973  | 4.267  | 1.00 | 37.51 | B |
| ATOM | 1697 | NH1  | ARG B | 34 | 50.622 | 0.003   | 4.729  | 1.00 | 39.45 | B |

| ATOM | 1698 | NH2 | ARG | B | 34 | 51.642 | -1.058 | 2.967 | 1.00 | 36.90 | B |
|------|------|-----|-----|---|----|--------|--------|-------|------|-------|---|
| ATOM | 1699 | C | ARG | B | 34 | 49.587 | -6.218 | 6.498 | 1.00 | 26.48 | B |
| ATOM | 1700 | O | ARG | B | 34 | 48.740 | -5.639 | 5.825 | 1.00 | 27.17 | B |
| ATOM | 1701 | N | GLU | B | 35 | 49.647 | -7.534 | 6.602 | 1.00 | 25.66 | B |
| ATOM | 1702 | CA | GLU | B | 35 | 48.746 | -8.394 | 5.867 | 1.00 | 26.99 | B |
| ATOM | 1703 | CB | GLU | B | 35 | 49.570 | -9.483 | 5.175 | 1.00 | 31.53 | B |
| ATOM | 1704 | CG | GLU | B | 35 | 48.814 | -10.396 | 4.235 | 1.00 | 36.29 | B |
| ATOM | 1705 | CD | GLU | B | 35 | 49.695 | -11.530 | 3.731 | 1.00 | 40.61 | B |
| ATOM | 1706 | OE1 | GLU | B | 35 | 50.825 | -11.240 | 3.276 | 1.00 | 45.20 | B |
| ATOM | 1707 | OE2 | GLU | B | 35 | 49.266 | -12.705 | 3.791 | 1.00 | 41.13 | B |
| ATOM | 1708 | C | GLU | B | 35 | 47.699 | -9.031 | 6.764 | 1.00 | 25.09 | B |
| ATOM | 1709 | O | GLU | B | 35 | 48.028 | -9.807 | 7.663 | 1.00 | 23.31 | B |
| ATOM | 1710 | N | GLU | B | 36 | 46.439 | -8.689 | 6.522 | 1.00 | 24.53 | B |
| ATOM | 1711 | CA | GLU | B | 36 | 45.332 | -9.263 | 7.275 | 1.00 | 25.73 | B |
| ATOM | 1712 | CB | GLU | B | 36 | 44.023 | -8.519 | 6.958 | 1.00 | 26.62 | B |
| ATOM | 1713 | CG | GLU | B | 36 | 42.783 | -9.095 | 7.636 | 1.00 | 28.26 | B |
| ATOM | 1714 | CD | GLU | B | 36 | 41.545 | -8.232 | 7.442 | 1.00 | 31.08 | B |
| ATOM | 1715 | OE1 | GLU | B | 36 | 41.420 | -7.590 | 6.377 | 1.00 | 32.56 | B |
| ATOM | 1716 | OE2 | GLU | B | 36 | 40.685 | -8.206 | 8.349 | 1.00 | 32.83 | B |
| ATOM | 1717 | C | GLU | B | 36 | 45.238 | -10.717 | 6.822 | 1.00 | 24.67 | B |
| ATOM | 1718 | O | GLU | B | 36 | 45.141 | -10.992 | 5.626 | 1.00 | 23.91 | B |
| ATOM | 1719 | N | ILE | B | 37 | 45.282 | -11.647 | 7.771 | 1.00 | 26.11 | B |
| ATOM | 1720 | CA | ILE | B | 37 | 45.219 | -13.067 | 7.433 | 1.00 | 27.80 | B |
| ATOM | 1721 | CB | ILE | B | 37 | 46.444 | -13.822 | 8.013 | 1.00 | 27.27 | B |
| ATOM | 1722 | CG2 | ILE | B | 37 | 47.728 | -13.174 | 7.516 | 1.00 | 27.41 | B |
| ATOM | 1723 | CG1 | ILE | B | 37 | 46.440 | -13.767 | 9.537 | 1.00 | 29.35 | B |
| ATOM | 1724 | CD1 | ILE | B | 37 | 47.596 | -14.509 | 10.175 | 1.00 | 30.27 | B |
| ATOM | 1725 | C | ILE | B | 37 | 43.922 | -13.750 | 7.879 | 1.00 | 27.86 | B |
| ATOM | 1726 | O | ILE | B | 37 | 43.445 | -14.674 | 7.221 | 1.00 | 28.29 | B |
| ATOM | 1727 | N | VAL | B | 38 | 43.348 | -13.296 | 8.989 | 1.00 | 28.78 | B |
| ATOM | 1728 | CA | VAL | B | 38 | 42.097 | -13.870 | 9.487 | 1.00 | 29.29 | B |
| ATOM | 1729 | CB | VAL | B | 38 | 42.294 | -14.751 | 10.741 | 1.00 | 30.18 | B |
| ATOM | 1730 | CG1 | VAL | B | 38 | 40.983 | -15.452 | 11.071 | 1.00 | 33.17 | B |
| ATOM | 1731 | CG2 | VAL | B | 38 | 43.399 | -15.764 | 10.520 | 1.00 | 31.09 | B |
| ATOM | 1732 | C | VAL | B | 38 | 41.161 | -12.745 | 9.882 | 1.00 | 28.75 | B |
| ATOM | 1733 | O | VAL | B | 38 | 41.585 | -11.758 | 10.480 | 1.00 | 29.70 | B |
| ATOM | 1734 | N | ARG | B | 39 | 39.881 | -12.911 | 9.581 | 1.00 | 27.05 | B |
| ATOM | 1735 | CA | ARG | B | 39 | 38.895 | -11.890 | 9.892 | 1.00 | 25.46 | B |
| ATOM | 1736 | CB | ARG | B | 39 | 38.627 | -11.064 | 8.632 | 1.00 | 27.23 | B |
| ATOM | 1737 | CG | ARG | B | 39 | 37.544 | -10.011 | 8.765 | 1.00 | 30.84 | B |
| ATOM | 1738 | CD | ARG | B | 39 | 37.111 | -9.476 | 7.398 | 1.00 | 29.34 | B |
| ATOM | 1739 | NE | ARG | B | 39 | 38.218 | -8.861 | 6.673 | 1.00 | 30.83 | B |
| ATOM | 1740 | CZ | ARG | B | 39 | 38.116 | -8.328 | 5.459 | 1.00 | 31.23 | B |
| ATOM | 1741 | NH1 | ARG | B | 39 | 36.951 | -8.333 | 4.823 | 1.00 | 31.08 | B |
| ATOM | 1742 | NH2 | ARG | B | 39 | 39.178 | -7.779 | 4.883 | 1.00 | 30.81 | B |
| ATOM | 1743 | C | ARG | B | 39 | 37.573 | -12.476 | 10.381 | 1.00 | 25.41 | B |
| ATOM | 1744 | O | ARG | B | 39 | 37.192 | -13.587 | 9.996 | 1.00 | 25.06 | B |
| ATOM | 1745 | N | PHE | B | 40 | 36.890 | -11.742 | 11.252 | 1.00 | 23.72 | B |
| ATOM | 1746 | CA | PHE | B | 40 | 35.569 | -12.164 | 11.696 | 1.00 | 24.04 | B |
| ATOM | 1747 | CB | PHE | B | 40 | 35.498 | -12.554 | 13.171 | 1.00 | 22.69 | B |
| ATOM | 1748 | CG | PHE | B | 40 | 34.133 | -13.036 | 13.573 | 1.00 | 20.75 | B |
| ATOM | 1749 | CD1 | PHE | B | 40 | 33.777 | -14.370 | 13.413 | 1.00 | 21.07 | B |
| ATOM | 1750 | CD2 | PHE | B | 40 | 33.162 | -12.135 | 14.003 | 1.00 | 21.00 | B |
| ATOM | 1751 | CE1 | PHE | B | 40 | 32.475 | -14.800 | 13.670 | 1.00 | 20.86 | B |
| ATOM | 1752 | CE2 | PHE | B | 40 | 31.858 | -12.553 | 14.261 | 1.00 | 19.95 | B |
| ATOM | 1753 | CZ | PHE | B | 40 | 31.517 | -13.890 | 14.092 | 1.00 | 19.78 | B |
| ATOM | 1754 | C | PHE | B | 40 | 34.662 | -10.969 | 11.474 | 1.00 | 24.27 | B |
| ATOM | 1755 | O | PHE | B | 40 | 34.755 | -9.970 | 12.183 | 1.00 | 22.94 | B |
| ATOM | 1756 | N | ASP | B | 41 | 33.800 | -11.088 | 10.471 | 1.00 | 24.75 | B |
| ATOM | 1757 | CA | ASP | B | 41 | 32.857 | -10.040 | 10.101 | 1.00 | 24.98 | B |
| ATOM | 1758 | CB | ASP | B | 41 | 32.863 | -9.881 | 8.578 | 1.00 | 25.64 | B |
| ATOM | 1759 | CG | ASP | B | 41 | 32.162 | -8.626 | 8.116 | 1.00 | 27.70 | B |
| ATOM | 1760 | OD1 | ASP | B | 41 | 31.163 | -8.227 | 8.749 | 1.00 | 26.21 | B |
| ATOM | 1761 | OD2 | ASP | B | 41 | 32.607 | -8.045 | 7.102 | 1.00 | 30.42 | B |
| ATOM | 1762 | C | ASP | B | 41 | 31.477 | -10.497 | 10.560 | 1.00 | 24.50 | B |
| ATOM | 1763 | O | ASP | B | 41 | 31.011 | -11.558 | 10.151 | 1.00 | 24.95 | B |
| ATOM | 1764 | N | SER | B | 42 | 30.822 | -9.710 | 11.404 | 1.00 | 24.16 | B |
| ATOM | 1765 | CA | SER | B | 42 | 29.501 | -10.096 | 11.882 | 1.00 | 26.13 | B |
| ATOM | 1766 | CB | SER | B | 42 | 29.013 | -9.133 | 12.972 | 1.00 | 24.53 | B |
| ATOM | 1767 | OG | SER | B | 42 | 28.932 | -7.806 | 12.497 | 1.00 | 23.39 | B |
| ATOM | 1768 | C | SER | B | 42 | 28.497 | -10.149 | 10.729 | 1.00 | 27.68 | B |
| ATOM | 1769 | O | SER | B | 42 | 27.474 | -10.833 | 10.818 | 1.00 | 27.31 | B |
| ATOM | 1770 | N | ASP | B | 43 | 28.789 | -9.419 | 9.654 | 1.00 | 28.17 | B |
| ATOM | 1771 | CA | ASP | B | 43 | 27.924 | -9.413 | 8.477 | 1.00 | 29.40 | B |

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ATOM   1772  CB  ASP B  43      28.332  -8.298   7.508  1.00 29.57      B
ATOM   1773  CG  ASP B  43      27.587  -7.006   7.766  1.00 32.71      B
ATOM   1774  OD1 ASP B  43      26.999  -6.868   8.862  1.00 33.94      B
ATOM   1775  OD2 ASP B  43      27.593  -6.120   6.881  1.00 33.98      B
ATOM   1776  C   ASP B  43      28.036 -10.762   7.782  1.00 29.46      B
ATOM   1777  O   ASP B  43      27.162 -11.150   7.009  1.00 30.77      B
ATOM   1778  N   VAL B  44      29.123 -11.471   8.068  1.00 27.98      B
ATOM   1779  CA  VAL B  44      29.365 -12.780   7.486  1.00 27.16      B
ATOM   1780  CB  VAL B  44      30.846 -12.939   7.075  1.00 27.32      B
ATOM   1781  CG1 VAL B  44      31.083 -14.323   6.488  1.00 24.09      B
ATOM   1782  CG2 VAL B  44      31.218 -11.857   6.073  1.00 24.66      B
ATOM   1783  C   VAL B  44      28.990 -13.867   8.490  1.00 28.43      B
ATOM   1784  O   VAL B  44      28.558 -14.948   8.108  1.00 29.45      B
ATOM   1785  N   GLY B  45      29.177 -13.590   9.774  1.00 28.05      B
ATOM   1786  CA  GLY B  45      28.794 -14.561  10.780  1.00 28.67      B
ATOM   1787  C   GLY B  45      29.758 -15.679  11.125  1.00 28.25      B
ATOM   1788  O   GLY B  45      29.458 -16.486  12.002  1.00 29.67      B
ATOM   1789  N   GLU B  46      30.895 -15.755  10.443  1.00 27.03      B
ATOM   1790  CA  GLU B  46      31.873 -16.787  10.757  1.00 29.26      B
ATOM   1791  CB  GLU B  46      31.571 -18.087  10.000  1.00 32.16      B
ATOM   1792  CG  GLU B  46      32.039 -18.121   8.554  1.00 37.36      B
ATOM   1793  CD  GLU B  46      31.752 -19.458   7.885  1.00 41.59      B
ATOM   1794  OE1 GLU B  46      32.163 -20.505   8.433  1.00 43.30      B
ATOM   1795  OE2 GLU B  46      31.116 -19.463   6.810  1.00 43.54      B
ATOM   1796  C   GLU B  46      33.272 -16.295  10.413  1.00 29.29      B
ATOM   1797  O   GLU B  46      33.432 -15.288   9.722  1.00 30.45      B
ATOM   1798  N   PHE B  47      34.281 -17.005  10.904  1.00 28.00      B
ATOM   1799  CA  PHE B  47      35.670 -16.650  10.651  1.00 28.10      B
ATOM   1800  CB  PHE B  47      36.594 -17.445  11.566  1.00 28.74      B
ATOM   1801  CG  PHE B  47      36.487 -17.067  13.016  1.00 30.23      B
ATOM   1802  CD1 PHE B  47      37.248 -16.023  13.535  1.00 28.96      B
ATOM   1803  CD2 PHE B  47      35.636 -17.768  13.870  1.00 30.80      B
ATOM   1804  CE1 PHE B  47      37.166 -15.683  14.888  1.00 31.59      B
ATOM   1805  CE2 PHE B  47      35.544 -17.435  15.229  1.00 31.97      B
ATOM   1806  CZ  PHE B  47      36.311 -16.392  15.737  1.00 30.36      B
ATOM   1807  C   PHE B  47      36.034 -16.948   9.211  1.00 28.71      B
ATOM   1808  O   PHE B  47      35.576 -17.937   8.640  1.00 28.03      B
ATOM   1809  N   ARG B  48      36.872 -16.091   8.637  1.00 27.96      B
ATOM   1810  CA  ARG B  48      37.327 -16.242   7.261  1.00 26.41      B
ATOM   1811  CB  ARG B  48      36.513 -15.341   6.326  1.00 26.57      B
ATOM   1812  CG  ARG B  48      35.068 -15.755   6.108  1.00 26.19      B
ATOM   1813  CD  ARG B  48      34.971 -17.079   5.352  1.00 24.98      B
ATOM   1814  NE  ARG B  48      33.579 -17.465   5.146  1.00 26.01      B
ATOM   1815  CZ  ARG B  48      32.755 -16.867   4.294  1.00 26.84      B
ATOM   1816  NH1 ARG B  48      33.181 -15.857   3.554  1.00 26.92      B
ATOM   1817  NH2 ARG B  48      31.492 -17.260   4.204  1.00 30.22      B
ATOM   1818  C   ARG B  48      38.799 -15.861   7.140  1.00 26.95      B
ATOM   1819  O   ARG B  48      39.255 -14.878   7.737  1.00 24.36      B
ATOM   1820  N   ALA B  49      39.542 -16.647   6.373  1.00 24.93      B
ATOM   1821  CA  ALA B  49      40.943 -16.349   6.143  1.00 26.58      B
ATOM   1822  CB  ALA B  49      41.709 -17.619   5.792  1.00 27.05      B
ATOM   1823  C   ALA B  49      40.927 -15.397   4.956  1.00 26.47      B
ATOM   1824  O   ALA B  49      40.210 -15.635   3.983  1.00 26.12      B
ATOM   1825  N   VAL B  50      41.674 -14.302   5.044  1.00 27.06      B
ATOM   1826  CA  VAL B  50      41.720 -13.357   3.936  1.00 26.50      B
ATOM   1827  CB  VAL B  50      41.790 -11.876   4.439  1.00 27.14      B
ATOM   1828  CG1 VAL B  50      42.327 -11.827   5.846  1.00 29.89      B
ATOM   1829  CG2 VAL B  50      42.628 -11.020   3.501  1.00 27.33      B
ATOM   1830  C   VAL B  50      42.891 -13.742   3.037  1.00 26.58      B
ATOM   1831  O   VAL B  50      42.914 -13.390   1.860  1.00 27.84      B
ATOM   1832  N   THR B  51      43.842 -14.489   3.598  1.00 26.61      B
ATOM   1833  CA  THR B  51      44.992 -15.011   2.846  1.00 28.59      B
ATOM   1834  CB  THR B  51      46.295 -14.193   3.056  1.00 28.25      B
ATOM   1835  OG1 THR B  51      46.828 -14.464   4.356  1.00 28.56      B
ATOM   1836  CG2 THR B  51      46.033 -12.699   2.899  1.00 27.40      B
ATOM   1837  C   THR B  51      45.256 -16.435   3.344  1.00 29.29      B
ATOM   1838  O   THR B  51      44.787 -16.818   4.418  1.00 30.16      B
ATOM   1839  N   LEU B  52      46.005 -17.217   2.575  1.00 30.64      B
ATOM   1840  CA  LEU B  52      46.309 -18.596   2.959  1.00 31.32      B
ATOM   1841  CB  LEU B  52      47.277 -19.237   1.963  1.00 32.19      B
ATOM   1842  CG  LEU B  52      46.706 -19.724   0.624  1.00 36.90      B
ATOM   1843  CD1 LEU B  52      47.836 -20.306  -0.216  1.00 35.68      B
ATOM   1844  CD2 LEU B  52      45.620 -20.775   0.861  1.00 35.34      B
ATOM   1845  C   LEU B  52      46.892 -18.724   4.359  1.00 31.57      B
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| ATOM | 1846 | O | LEU B | 52 | 46.570 -19.656 | 5.097 | 1.00 31.50 | B |
|------|------|-----|-------|----|----|----|----|----|
| ATOM | 1847 | N | LEU B | 53 | 47.753 -17.786 | 4.723 | 1.00 31.09 | B |
| ATOM | 1848 | CA | LEU B | 53 | 48.388 -17.815 | 6.029 | 1.00 30.93 | B |
| ATOM | 1849 | CB | LEU B | 53 | 49.160 -16.511 | 6.246 | 1.00 31.99 | B |
| ATOM | 1850 | CG | LEU B | 53 | 50.338 -16.532 | 7.221 | 1.00 35.20 | B |
| ATOM | 1851 | CD1 | LEU B | 53 | 51.364 -17.559 | 6.763 | 1.00 35.92 | B |
| ATOM | 1852 | CD2 | LEU B | 53 | 50.975 -15.148 | 7.284 | 1.00 34.96 | B |
| ATOM | 1853 | C | LEU B | 53 | 47.377 -18.017 | 7.160 | 1.00 29.90 | B |
| ATOM | 1854 | O | LEU B | 53 | 47.663 -18.709 | 8.138 | 1.00 30.68 | B |
| ATOM | 1855 | N | GLY B | 54 | 46.192 -17.430 | 7.015 | 1.00 28.63 | B |
| ATOM | 1856 | CA | GLY B | 54 | 45.181 -17.537 | 8.057 | 1.00 29.75 | B |
| ATOM | 1857 | C | GLY B | 54 | 44.140 -18.635 | 7.901 | 1.00 30.44 | B |
| ATOM | 1858 | O | GLY B | 54 | 43.146 -18.664 | 8.630 | 1.00 28.02 | B |
| ATOM | 1859 | N | LEU B | 55 | 44.364 -19.547 | 6.964 | 1.00 30.54 | B |
| ATOM | 1860 | CA | LEU B | 55 | 43.417 -20.630 | 6.732 | 1.00 32.59 | B |
| ATOM | 1861 | CB | LEU B | 55 | 43.765 -21.344 | 5.422 | 1.00 35.94 | B |
| ATOM | 1862 | CG | LEU B | 55 | 42.776 -22.383 | 4.889 | 1.00 38.88 | B |
| ATOM | 1863 | CD1 | LEU B | 55 | 41.355 -21.831 | 4.927 | 1.00 38.23 | B |
| ATOM | 1864 | CD2 | LEU B | 55 | 43.173 -22.766 | 3.467 | 1.00 39.03 | B |
| ATOM | 1865 | C | LEU B | 55 | 43.330 -21.631 | 7.892 | 1.00 32.20 | B |
| ATOM | 1866 | O | LEU B | 55 | 42.235 -22.026 | 8.291 | 1.00 33.32 | B |
| ATOM | 1867 | N | PRO B | 56 | 44.478 -22.058 | 8.447 | 1.00 31.03 | B |
| ATOM | 1868 | CD | PRO B | 56 | 45.862 -21.802 | 8.009 | 1.00 30.17 | B |
| ATOM | 1869 | CA | PRO B | 56 | 44.451 -23.013 | 9.561 | 1.00 30.23 | B |
| ATOM | 1870 | CB | PRO B | 56 | 45.925 -23.148 | 9.931 | 1.00 30.27 | B |
| ATOM | 1871 | CG | PRO B | 56 | 46.609 -22.967 | 8.610 | 1.00 28.92 | B |
| ATOM | 1872 | C | PRO B | 56 | 43.613 -22.525 | 10.740 | 1.00 31.42 | B |
| ATOM | 1873 | O | PRO B | 56 | 42.730 -23.237 | 11.222 | 1.00 33.17 | B |
| ATOM | 1874 | N | ALA B | 57 | 43.893 -21.305 | 11.196 | 1.00 30.04 | B |
| ATOM | 1875 | CA | ALA B | 57 | 43.181 -20.719 | 12.322 | 1.00 28.60 | B |
| ATOM | 1876 | CB | ALA B | 57 | 43.818 -19.389 | 12.697 | 1.00 26.81 | B |
| ATOM | 1877 | C | ALA B | 57 | 41.695 -20.528 | 12.021 | 1.00 29.08 | B |
| ATOM | 1878 | O | ALA B | 57 | 40.847 -20.737 | 12.887 | 1.00 28.22 | B |
| ATOM | 1879 | N | ALA B | 58 | 41.385 -20.135 | 10.791 | 1.00 28.84 | B |
| ATOM | 1880 | CA | ALA B | 58 | 40.002 -19.922 | 10.386 | 1.00 31.06 | B |
| ATOM | 1881 | CB | ALA B | 58 | 39.955 -19.426 | 8.947 | 1.00 29.79 | B |
| ATOM | 1882 | C | ALA B | 58 | 39.169 -21.199 | 10.529 | 1.00 32.38 | B |
| ATOM | 1883 | O | ALA B | 58 | 38.113 -21.197 | 11.170 | 1.00 31.57 | B |
| ATOM | 1884 | N | GLU B | 59 | 39.647 -22.285 | 9.929 | 1.00 33.50 | B |
| ATOM | 1885 | CA | GLU B | 59 | 38.949 -23.565 | 9.993 | 1.00 33.91 | B |
| ATOM | 1886 | CB | GLU B | 59 | 39.706 -24.622 | 9.195 | 1.00 35.67 | B |
| ATOM | 1887 | CG | GLU B | 59 | 39.619 -24.457 | 7.696 | 1.00 39.73 | B |
| ATOM | 1888 | CD | GLU B | 59 | 40.327 -25.583 | 6.957 | 1.00 43.58 | B |
| ATOM | 1889 | OE1 | GLU B | 59 | 41.561 -25.715 | 7.119 | 1.00 44.52 | B |
| ATOM | 1890 | OE2 | GLU B | 59 | 39.648 -26.337 | 6.222 | 1.00 44.30 | B |
| ATOM | 1891 | C | GLU B | 59 | 38.771 -24.063 | 11.425 | 1.00 33.56 | B |
| ATOM | 1892 | O | GLU B | 59 | 37.708 -24.570 | 11.790 | 1.00 34.40 | B |
| ATOM | 1893 | N | TYR B | 60 | 39.815 -23.923 | 12.233 | 1.00 31.99 | B |
| ATOM | 1894 | CA | TYR B | 60 | 39.754 -24.369 | 13.611 | 1.00 31.01 | B |
| ATOM | 1895 | CB | TYR B | 60 | 41.112 -24.202 | 14.292 | 1.00 31.13 | B |
| ATOM | 1896 | CG | TYR B | 60 | 41.051 -24.548 | 15.750 | 1.00 30.99 | B |
| ATOM | 1897 | CD1 | TYR B | 60 | 40.919 -25.871 | 16.162 | 1.00 32.55 | B |
| ATOM | 1898 | CE1 | TYR B | 60 | 40.770 -26.192 | 17.508 | 1.00 35.39 | B |
| ATOM | 1899 | CD2 | TYR B | 60 | 41.039 -23.550 | 16.716 | 1.00 32.67 | B |
| ATOM | 1900 | CE2 | TYR B | 60 | 40.890 -23.853 | 18.064 | 1.00 35.14 | B |
| ATOM | 1901 | CZ | TYR B | 60 | 40.756 -25.177 | 18.455 | 1.00 36.91 | B |
| ATOM | 1902 | OH | TYR B | 60 | 40.606 -25.483 | 19.791 | 1.00 40.06 | B |
| ATOM | 1903 | C | TYR B | 60 | 38.695 -23.631 | 14.426 | 1.00 31.72 | B |
| ATOM | 1904 | O | TYR B | 60 | 37.840 -24.258 | 15.050 | 1.00 31.72 | B |
| ATOM | 1905 | N | TRP B | 61 | 38.752 -22.303 | 14.428 | 1.00 30.37 | B |
| ATOM | 1906 | CA | TRP B | 61 | 37.790 -21.525 | 15.194 | 1.00 31.57 | B |
| ATOM | 1907 | CB | TRP B | 61 | 38.129 -20.024 | 15.140 | 1.00 32.14 | B |
| ATOM | 1908 | CG | TRP B | 61 | 39.430 -19.666 | 15.824 | 1.00 33.73 | B |
| ATOM | 1909 | CD2 | TRP B | 61 | 40.359 -18.648 | 15.429 | 1.00 35.16 | B |
| ATOM | 1910 | CE2 | TRP B | 61 | 41.418 -18.662 | 16.362 | 1.00 35.99 | B |
| ATOM | 1911 | CE3 | TRP B | 61 | 40.397 -17.719 | 14.378 | 1.00 38.30 | B |
| ATOM | 1912 | CD1 | TRP B | 61 | 39.949 -20.236 | 16.949 | 1.00 33.63 | B |
| ATOM | 1913 | NE1 | TRP B | 61 | 41.142 -19.642 | 17.278 | 1.00 33.97 | B |
| ATOM | 1914 | CZ2 | TRP B | 61 | 42.512 -17.782 | 16.277 | 1.00 38.13 | B |
| ATOM | 1915 | CZ3 | TRP B | 61 | 41.487 -16.836 | 14.293 | 1.00 39.26 | B |
| ATOM | 1916 | CH2 | TRP B | 61 | 42.527 -16.879 | 15.240 | 1.00 38.22 | B |
| ATOM | 1917 | C | TRP B | 61 | 36.349 -21.758 | 14.739 | 1.00 31.22 | B |
| ATOM | 1918 | O | TRP B | 61 | 35.436 -21.758 | 15.559 | 1.00 29.98 | B |
| ATOM | 1919 | N | ASN B | 62 | 36.137 -21.955 | 13.440 | 1.00 31.63 | B |

| ATOM | 1920 | CA | ASN | B | 62 | 34.781 | -22.191 | 12.950 | 1.00 | 32.57 | B |
|------|------|-----|-----|---|----|--------|---------|--------|------|-------|---|
| ATOM | 1921 | CB | ASN | B | 62 | 34.701 | -22.021 | 11.434 | 1.00 | 30.37 | B |
| ATOM | 1922 | CG | ASN | B | 62 | 34.575 | -20.574 | 11.025 | 1.00 | 29.69 | B |
| ATOM | 1923 | OD1 | ASN | B | 62 | 33.889 | -19.794 | 11.680 | 1.00 | 29.42 | B |
| ATOM | 1924 | ND2 | ASN | B | 62 | 35.222 | -20.209 | 9.926 | 1.00 | 31.50 | B |
| ATOM | 1925 | C | ASN | B | 62 | 34.238 | -23.561 | 13.339 | 1.00 | 32.87 | B |
| ATOM | 1926 | O | ASN | B | 62 | 33.028 | -23.789 | 13.292 | 1.00 | 34.70 | B |
| ATOM | 1927 | N | SER | B | 63 | 35.128 | -24.469 | 13.725 | 1.00 | 32.43 | B |
| ATOM | 1928 | CA | SER | B | 63 | 34.705 | -25.797 | 14.140 | 1.00 | 32.38 | B |
| ATOM | 1929 | CB | SER | B | 63 | 35.818 | -26.819 | 13.879 | 1.00 | 32.20 | B |
| ATOM | 1930 | OG | SER | B | 63 | 36.905 | -26.626 | 14.760 | 1.00 | 33.33 | B |
| ATOM | 1931 | C | SER | B | 63 | 34.348 | -25.768 | 15.630 | 1.00 | 32.14 | B |
| ATOM | 1932 | O | SER | B | 63 | 33.677 | -26.667 | 16.138 | 1.00 | 32.86 | B |
| ATOM | 1933 | N | GLN | B | 64 | 34.794 | -24.724 | 16.325 | 1.00 | 31.10 | B |
| ATOM | 1934 | CA | GLN | B | 64 | 34.513 | -24.569 | 17.752 | 1.00 | 30.99 | B |
| ATOM | 1935 | CB | GLN | B | 64 | 35.661 | -23.837 | 18.446 | 1.00 | 32.54 | B |
| ATOM | 1936 | CG | GLN | B | 64 | 36.988 | -24.557 | 18.383 | 1.00 | 34.49 | B |
| ATOM | 1937 | CD | GLN | B | 64 | 36.870 | -25.998 | 18.810 | 1.00 | 38.20 | B |
| ATOM | 1938 | OE1 | GLN | B | 64 | 36.629 | -26.884 | 17.984 | 1.00 | 40.82 | B |
| ATOM | 1939 | NE2 | GLN | B | 64 | 37.022 | -26.245 | 20.108 | 1.00 | 38.34 | B |
| ATOM | 1940 | C | GLN | B | 64 | 33.226 | -23.775 | 17.944 | 1.00 | 29.88 | B |
| ATOM | 1941 | O | GLN | B | 64 | 33.252 | -22.549 | 18.064 | 1.00 | 29.28 | B |
| ATOM | 1942 | N | LYS | B | 65 | 32.101 | -24.476 | 17.979 | 1.00 | 28.74 | B |
| ATOM | 1943 | CA | LYS | B | 65 | 30.815 | -23.812 | 18.123 | 1.00 | 29.18 | B |
| ATOM | 1944 | CB | LYS | B | 65 | 29.688 | -24.851 | 18.132 | 1.00 | 30.63 | B |
| ATOM | 1945 | CG | LYS | B | 65 | 29.575 | -25.612 | 16.812 | 1.00 | 32.20 | B |
| ATOM | 1946 | CD | LYS | B | 65 | 29.371 | -24.654 | 15.629 | 1.00 | 34.44 | B |
| ATOM | 1947 | CE | LYS | B | 65 | 29.688 | -25.327 | 14.284 | 1.00 | 37.24 | B |
| ATOM | 1948 | NZ | LYS | B | 65 | 29.430 | -24.427 | 13.109 | 1.00 | 37.89 | B |
| ATOM | 1949 | C | LYS | B | 65 | 30.745 | -22.919 | 19.352 | 1.00 | 28.19 | B |
| ATOM | 1950 | O | LYS | B | 65 | 30.075 | -21.891 | 19.333 | 1.00 | 28.16 | B |
| ATOM | 1951 | N | ASP | B | 66 | 31.440 | -23.304 | 20.417 | 1.00 | 27.58 | B |
| ATOM | 1952 | CA | ASP | B | 66 | 31.460 | -22.504 | 21.636 | 1.00 | 27.41 | B |
| ATOM | 1953 | CB | ASP | B | 66 | 32.283 | -23.208 | 22.727 | 1.00 | 28.45 | B |
| ATOM | 1954 | CG | ASP | B | 66 | 33.559 | -23.847 | 22.184 | 1.00 | 32.24 | B |
| ATOM | 1955 | OD1 | ASP | B | 66 | 33.478 | -24.591 | 21.183 | 1.00 | 33.17 | B |
| ATOM | 1956 | OD2 | ASP | B | 66 | 34.642 | -23.623 | 22.765 | 1.00 | 33.25 | B |
| ATOM | 1957 | C | ASP | B | 66 | 32.050 | -21.131 | 21.316 | 1.00 | 26.63 | B |
| ATOM | 1958 | O | ASP | B | 66 | 31.468 | -20.102 | 21.662 | 1.00 | 24.32 | B |
| ATOM | 1959 | N | ILE | B | 67 | 33.198 | -21.116 | 20.640 | 1.00 | 26.12 | B |
| ATOM | 1960 | CA | ILE | B | 67 | 33.840 | -19.855 | 20.273 | 1.00 | 26.42 | B |
| ATOM | 1961 | CB | ILE | B | 67 | 35.206 | -20.088 | 19.613 | 1.00 | 28.29 | B |
| ATOM | 1962 | CG2 | ILE | B | 67 | 35.859 | -18.753 | 19.290 | 1.00 | 28.54 | B |
| ATOM | 1963 | CG1 | ILE | B | 67 | 36.094 | -20.925 | 20.535 | 1.00 | 28.25 | B |
| ATOM | 1964 | CD1 | ILE | B | 67 | 36.319 | -20.321 | 21.906 | 1.00 | 32.66 | B |
| ATOM | 1965 | C | ILE | B | 67 | 32.968 | -19.061 | 19.300 | 1.00 | 26.36 | B |
| ATOM | 1966 | O | ILE | B | 67 | 32.747 | -17.869 | 19.491 | 1.00 | 25.33 | B |
| ATOM | 1967 | N | LEU | B | 68 | 32.472 | -19.730 | 18.261 | 1.00 | 26.11 | B |
| ATOM | 1968 | CA | LEU | B | 68 | 31.617 | -19.086 | 17.267 | 1.00 | 26.66 | B |
| ATOM | 1969 | CB | LEU | B | 68 | 31.132 | -20.102 | 16.235 | 1.00 | 27.61 | B |
| ATOM | 1970 | CG | LEU | B | 68 | 31.807 | -20.171 | 14.872 | 1.00 | 30.12 | B |
| ATOM | 1971 | CD1 | LEU | B | 68 | 31.081 | -21.216 | 14.031 | 1.00 | 33.09 | B |
| ATOM | 1972 | CD2 | LEU | B | 68 | 31.766 | -18.812 | 14.190 | 1.00 | 30.01 | B |
| ATOM | 1973 | C | LEU | B | 68 | 30.394 | -18.415 | 17.878 | 1.00 | 26.81 | B |
| ATOM | 1974 | O | LEU | B | 68 | 30.067 | -17.280 | 17.541 | 1.00 | 26.19 | B |
| ATOM | 1975 | N | GLU | B | 69 | 29.706 | -19.135 | 18.756 | 1.00 | 28.87 | B |
| ATOM | 1976 | CA | GLU | B | 69 | 28.509 | -18.614 | 19.404 | 1.00 | 31.55 | B |
| ATOM | 1977 | CB | GLU | B | 69 | 27.945 | -19.654 | 20.382 | 1.00 | 35.75 | B |
| ATOM | 1978 | CG | GLU | B | 69 | 27.304 | -20.862 | 19.695 | 1.00 | 43.71 | B |
| ATOM | 1979 | CD | GLU | B | 69 | 26.883 | -21.954 | 20.673 | 1.00 | 47.92 | B |
| ATOM | 1980 | OE1 | GLU | B | 69 | 27.756 | -22.454 | 21.418 | 1.00 | 49.27 | B |
| ATOM | 1981 | OE2 | GLU | B | 69 | 25.683 | -22.316 | 20.694 | 1.00 | 50.44 | B |
| ATOM | 1982 | C | GLU | B | 69 | 28.773 | -17.295 | 20.130 | 1.00 | 29.82 | B |
| ATOM | 1983 | O | GLU | B | 69 | 27.986 | -16.356 | 20.027 | 1.00 | 27.91 | B |
| ATOM | 1984 | N | ARG | B | 70 | 29.886 | -17.226 | 20.855 | 1.00 | 29.32 | B |
| ATOM | 1985 | CA | ARG | B | 70 | 30.239 | -16.016 | 21.597 | 1.00 | 28.97 | B |
| ATOM | 1986 | CB | ARG | B | 70 | 31.347 | -16.315 | 22.606 | 1.00 | 28.94 | B |
| ATOM | 1987 | CG | ARG | B | 70 | 30.982 | -17.344 | 23.673 | 1.00 | 30.55 | B |
| ATOM | 1988 | CD | ARG | B | 70 | 32.251 | -17.810 | 24.371 | 1.00 | 32.35 | B |
| ATOM | 1989 | NE | ARG | B | 70 | 32.040 | -19.037 | 25.117 | 1.00 | 34.83 | B |
| ATOM | 1990 | CZ | ARG | B | 70 | 32.946 | -19.997 | 25.232 | 1.00 | 34.98 | B |
| ATOM | 1991 | NH1 | ARG | B | 70 | 34.131 | -19.875 | 24.647 | 1.00 | 35.03 | B |
| ATOM | 1992 | NH2 | ARG | B | 70 | 32.662 | -21.083 | 25.930 | 1.00 | 39.48 | B |
| ATOM | 1993 | C | ARG | B | 70 | 30.691 | -14.888 | 20.682 | 1.00 | 26.77 | B |

| ATOM | 1994 | O | ARG | B | 70 | 30.412 | -13.725 | 20.951 | 1.00 | 26.95 | B |
| ATOM | 1995 | N | LYS | B | 71 | 31.395 | -15.235 | 19.608 | 1.00 | 25.97 | B |
| ATOM | 1996 | CA | LYS | B | 71 | 31.885 | -14.236 | 18.670 | 1.00 | 25.98 | B |
| ATOM | 1997 | CB | LYS | B | 71 | 32.830 | -14.877 | 17.652 | 1.00 | 27.62 | B |
| ATOM | 1998 | CG | LYS | B | 71 | 33.728 | -13.873 | 16.924 | 1.00 | 29.24 | B |
| ATOM | 1999 | CD | LYS | B | 71 | 34.628 | -13.137 | 17.909 | 1.00 | 32.14 | B |
| ATOM | 2000 | CE | LYS | B | 71 | 35.430 | -12.035 | 17.236 | 1.00 | 33.13 | B |
| ATOM | 2001 | NZ | LYS | B | 71 | 36.093 | -11.164 | 18.245 | 1.00 | 34.18 | B |
| ATOM | 2002 | C | LYS | B | 71 | 30.710 | -13.591 | 17.952 | 1.00 | 25.22 | B |
| ATOM | 2003 | O | LYS | B | 71 | 30.719 | -12.395 | 17.671 | 1.00 | 24.39 | B |
| ATOM | 2004 | N | ARG | B | 72 | 29.701 | -14.399 | 17.657 | 1.00 | 25.08 | B |
| ATOM | 2005 | CA | ARG | B | 72 | 28.500 | -13.922 | 16.989 | 1.00 | 26.32 | B |
| ATOM | 2006 | CB | ARG | B | 72 | 27.628 | -15.101 | 16.561 | 1.00 | 28.02 | B |
| ATOM | 2007 | CG | ARG | B | 72 | 28.116 | -15.830 | 15.340 | 1.00 | 28.10 | B |
| ATOM | 2008 | CD | ARG | B | 72 | 27.225 | -17.013 | 15.083 | 1.00 | 32.02 | B |
| ATOM | 2009 | NE | ARG | B | 72 | 27.451 | -17.583 | 13.766 | 1.00 | 36.46 | B |
| ATOM | 2010 | CZ | ARG | B | 72 | 27.014 | -18.779 | 13.389 | 1.00 | 38.62 | B |
| ATOM | 2011 | NH1 | ARG | B | 72 | 26.324 | -19.538 | 14.238 | 1.00 | 37.88 | B |
| ATOM | 2012 | NH2 | ARG | B | 72 | 27.270 | -19.212 | 12.163 | 1.00 | 38.55 | B |
| ATOM | 2013 | C | ARG | B | 72 | 27.687 | -13.017 | 17.898 | 1.00 | 24.31 | B |
| ATOM | 2014 | O | ARG | B | 72 | 26.792 | -12.326 | 17.439 | 1.00 | 24.84 | B |
| ATOM | 2015 | N | ALA | B | 73 | 27.990 | -13.028 | 19.189 | 1.00 | 26.18 | B |
| ATOM | 2016 | CA | ALA | B | 73 | 27.267 | -12.185 | 20.140 | 1.00 | 28.18 | B |
| ATOM | 2017 | CB | ALA | B | 73 | 26.973 | -12.974 | 21.418 | 1.00 | 28.97 | B |
| ATOM | 2018 | C | ALA | B | 73 | 28.056 | -10.916 | 20.472 | 1.00 | 28.97 | B |
| ATOM | 2019 | O | ALA | B | 73 | 27.528 | -9.977 | 21.066 | 1.00 | 30.50 | B |
| ATOM | 2020 | N | ALA | B | 74 | 29.320 | -10.882 | 20.070 | 1.00 | 29.65 | B |
| ATOM | 2021 | CA | ALA | B | 74 | 30.170 | -9.732 | 20.347 | 1.00 | 30.77 | B |
| ATOM | 2022 | CB | ALA | B | 74 | 31.558 | -9.966 | 19.764 | 1.00 | 30.77 | B |
| ATOM | 2023 | C | ALA | B | 74 | 29.594 | -8.414 | 19.827 | 1.00 | 31.78 | B |
| ATOM | 2024 | O | ALA | B | 74 | 29.789 | -7.359 | 20.438 | 1.00 | 32.74 | B |
| ATOM | 2025 | N | VAL | B | 75 | 28.886 | -8.465 | 18.704 | 1.00 | 31.60 | B |
| ATOM | 2026 | CA | VAL | B | 75 | 28.308 | -7.248 | 18.145 | 1.00 | 32.38 | B |
| ATOM | 2027 | CB | VAL | B | 75 | 27.397 | -7.539 | 16.929 | 1.00 | 30.51 | B |
| ATOM | 2028 | CG1 | VAL | B | 75 | 27.291 | -6.295 | 16.062 | 1.00 | 31.44 | B |
| ATOM | 2029 | CG2 | VAL | B | 75 | 27.931 | -8.696 | 16.137 | 1.00 | 33.08 | B |
| ATOM | 2030 | C | VAL | B | 75 | 27.465 | -6.529 | 19.201 | 1.00 | 33.07 | B |
| ATOM | 2031 | O | VAL | B | 75 | 27.402 | -5.302 | 19.218 | 1.00 | 33.54 | B |
| ATOM | 2032 | N | ASP | B | 76 | 26.811 | -7.302 | 20.065 | 1.00 | 34.70 | B |
| ATOM | 2033 | CA | ASP | B | 76 | 25.971 | -6.748 | 21.130 | 1.00 | 36.27 | B |
| ATOM | 2034 | CB | ASP | B | 76 | 24.780 | -7.670 | 21.420 | 1.00 | 38.57 | B |
| ATOM | 2035 | CG | ASP | B | 76 | 23.889 | -7.881 | 20.215 | 1.00 | 41.48 | B |
| ATOM | 2036 | OD1 | ASP | B | 76 | 23.335 | -6.887 | 19.694 | 1.00 | 43.46 | B |
| ATOM | 2037 | OD2 | ASP | B | 76 | 23.739 | -9.048 | 19.792 | 1.00 | 43.76 | B |
| ATOM | 2038 | C | ASP | B | 76 | 26.780 | -6.600 | 22.411 | 1.00 | 35.56 | B |
| ATOM | 2039 | O | ASP | B | 76 | 26.731 | -5.569 | 23.081 | 1.00 | 34.13 | B |
| ATOM | 2040 | N | ARG | B | 77 | 27.508 | -7.661 | 22.744 | 1.00 | 35.22 | B |
| ATOM | 2041 | CA | ARG | B | 77 | 28.343 | -7.708 | 23.937 | 1.00 | 34.49 | B |
| ATOM | 2042 | CB | ARG | B | 77 | 29.071 | -9.052 | 23.991 | 1.00 | 37.16 | B |
| ATOM | 2043 | CG | ARG | B | 77 | 29.841 | -9.328 | 25.271 | 1.00 | 40.90 | B |
| ATOM | 2044 | CD | ARG | B | 77 | 30.735 | -10.553 | 25.102 | 1.00 | 43.79 | B |
| ATOM | 2045 | NE | ARG | B | 77 | 30.004 | -11.743 | 24.665 | 1.00 | 48.65 | B |
| ATOM | 2046 | CZ | ARG | B | 77 | 29.103 | -12.385 | 25.406 | 1.00 | 51.36 | B |
| ATOM | 2047 | NH1 | ARG | B | 77 | 28.816 | -11.949 | 26.626 | 1.00 | 52.34 | B |
| ATOM | 2048 | NH2 | ARG | B | 77 | 28.499 | -13.470 | 24.935 | 1.00 | 50.76 | B |
| ATOM | 2049 | C | ARG | B | 77 | 29.362 | -6.576 | 23.927 | 1.00 | 32.18 | B |
| ATOM | 2050 | O | ARG | B | 77 | 29.499 | -5.835 | 24.896 | 1.00 | 32.49 | B |
| ATOM | 2051 | N | VAL | B | 78 | 30.073 | -6.442 | 22.818 | 1.00 | 30.66 | B |
| ATOM | 2052 | CA | VAL | B | 78 | 31.086 | -5.414 | 22.707 | 1.00 | 29.00 | B |
| ATOM | 2053 | CB | VAL | B | 78 | 32.276 | -5.917 | 21.867 | 1.00 | 27.82 | B |
| ATOM | 2054 | CG1 | VAL | B | 78 | 33.327 | -4.815 | 21.740 | 1.00 | 25.08 | B |
| ATOM | 2055 | CG2 | VAL | B | 78 | 32.870 | -7.160 | 22.504 | 1.00 | 23.27 | B |
| ATOM | 2056 | C | VAL | B | 78 | 30.594 | -4.093 | 22.113 | 1.00 | 29.33 | B |
| ATOM | 2057 | O | VAL | B | 78 | 30.435 | -3.104 | 22.831 | 1.00 | 29.83 | B |
| ATOM | 2058 | N | CYS | B | 79 | 30.354 | -4.091 | 20.804 | 1.00 | 28.42 | B |
| ATOM | 2059 | CA | CYS | B | 79 | 29.927 | -2.891 | 20.083 | 1.00 | 29.14 | B |
| ATOM | 2060 | C | CYS | B | 79 | 28.724 | -2.107 | 20.629 | 1.00 | 28.59 | B |
| ATOM | 2061 | O | CYS | B | 79 | 28.883 | -0.961 | 21.062 | 1.00 | 26.06 | B |
| ATOM | 2062 | CB | CYS | B | 79 | 29.675 | -3.219 | 18.604 | 1.00 | 29.19 | B |
| ATOM | 2063 | SG | CYS | B | 79 | 31.052 | -3.983 | 17.680 | 1.00 | 31.71 | B |
| ATOM | 2064 | N | ARG | B | 80 | 27.527 | -2.693 | 20.586 | 1.00 | 28.34 | B |
| ATOM | 2065 | CA | ARG | B | 80 | 26.347 | -1.980 | 21.071 | 1.00 | 30.77 | B |
| ATOM | 2066 | CB | ARG | B | 80 | 25.079 | -2.828 | 20.915 | 1.00 | 32.82 | B |
| ATOM | 2067 | CG | ARG | B | 80 | 24.612 | -2.973 | 19.474 | 1.00 | 35.65 | B |

| ATOM | 2068 | CD | ARG | B | 80 | 23.120 | -3.273 | 19.387 | 1.00 | 36.01 | B |
| ATOM | 2069 | NE | ARG | B | 80 | 22.649 | -3.243 | 18.005 | 1.00 | 35.49 | B |
| ATOM | 2070 | CZ | ARG | B | 80 | 22.913 | -4.188 | 17.108 | 1.00 | 37.80 | B |
| ATOM | 2071 | NH1 | ARG | B | 80 | 23.640 | -5.242 | 17.449 | 1.00 | 40.57 | B |
| ATOM | 2072 | NH2 | ARG | B | 80 | 22.467 | -4.075 | 15.864 | 1.00 | 38.86 | B |
| ATOM | 2073 | C | ARG | B | 80 | 26.507 | -1.552 | 22.524 | 1.00 | 31.24 | B |
| ATOM | 2074 | O | ARG | B | 80 | 25.975 | -0.525 | 22.944 | 1.00 | 32.07 | B |
| ATOM | 2075 | N | HIS | B | 81 | 27.257 | -2.337 | 23.283 | 1.00 | 31.40 | B |
| ATOM | 2076 | CA | HIS | B | 81 | 27.492 | -2.028 | 24.683 | 1.00 | 32.20 | B |
| ATOM | 2077 | CB | HIS | B | 81 | 28.220 | -3.185 | 25.366 | 1.00 | 33.00 | B |
| ATOM | 2078 | CG | HIS | B | 81 | 28.595 | -2.899 | 26.787 | 1.00 | 37.24 | B |
| ATOM | 2079 | CD2 | HIS | B | 81 | 29.764 | -2.490 | 27.335 | 1.00 | 38.05 | B |
| ATOM | 2080 | ND1 | HIS | B | 81 | 27.692 | -2.981 | 27.826 | 1.00 | 39.11 | B |
| ATOM | 2081 | CE1 | HIS | B | 81 | 28.290 | -2.635 | 28.952 | 1.00 | 40.49 | B |
| ATOM | 2082 | NE2 | HIS | B | 81 | 29.548 | -2.332 | 28.682 | 1.00 | 39.16 | B |
| ATOM | 2083 | C | HIS | B | 81 | 28.326 | -0.762 | 24.831 | 1.00 | 30.87 | B |
| ATOM | 2084 | O | HIS | B | 81 | 27.906 | 0.206 | 25.470 | 1.00 | 31.38 | B |
| ATOM | 2085 | N | ASN | B | 82 | 29.511 | -0.770 | 24.233 | 1.00 | 29.77 | B |
| ATOM | 2086 | CA | ASN | B | 82 | 30.403 | 0.375 | 24.332 | 1.00 | 28.02 | B |
| ATOM | 2087 | CB | ASN | B | 82 | 31.755 | 0.056 | 23.683 | 1.00 | 26.64 | B |
| ATOM | 2088 | CG | ASN | B | 82 | 32.470 | -1.092 | 24.373 | 1.00 | 25.02 | B |
| ATOM | 2089 | OD1 | ASN | B | 82 | 32.305 | -1.305 | 25.572 | 1.00 | 24.06 | B |
| ATOM | 2090 | ND2 | ASN | B | 82 | 33.278 | -1.829 | 23.619 | 1.00 | 26.38 | B |
| ATOM | 2091 | C | ASN | B | 82 | 29.819 | 1.648 | 23.741 | 1.00 | 26.04 | B |
| ATOM | 2092 | O | ASN | B | 82 | 30.163 | 2.747 | 24.174 | 1.00 | 25.71 | B |
| ATOM | 2093 | N | TYR | B | 83 | 28.930 | 1.512 | 22.765 | 1.00 | 25.90 | B |
| ATOM | 2094 | CA | TYR | B | 83 | 28.324 | 2.693 | 22.156 | 1.00 | 25.91 | B |
| ATOM | 2095 | CB | TYR | B | 83 | 27.462 | 2.297 | 20.946 | 1.00 | 25.69 | B |
| ATOM | 2096 | CG | TYR | B | 83 | 27.102 | 3.462 | 20.056 | 1.00 | 25.95 | B |
| ATOM | 2097 | CD1 | TYR | B | 83 | 26.022 | 4.294 | 20.353 | 1.00 | 27.11 | B |
| ATOM | 2098 | CE1 | TYR | B | 83 | 25.712 | 5.403 | 19.545 | 1.00 | 25.98 | B |
| ATOM | 2099 | CD2 | TYR | B | 83 | 27.865 | 3.759 | 18.933 | 1.00 | 27.72 | B |
| ATOM | 2100 | CE2 | TYR | B | 83 | 27.567 | 4.862 | 18.121 | 1.00 | 28.05 | B |
| ATOM | 2101 | CZ | TYR | B | 83 | 26.493 | 5.680 | 18.434 | 1.00 | 27.73 | B |
| ATOM | 2102 | OH | TYR | B | 83 | 26.225 | 6.781 | 17.645 | 1.00 | 27.55 | B |
| ATOM | 2103 | C | TYR | B | 83 | 27.485 | 3.458 | 23.181 | 1.00 | 25.87 | B |
| ATOM | 2104 | O | TYR | B | 83 | 27.315 | 4.673 | 23.070 | 1.00 | 26.05 | B |
| ATOM | 2105 | N | GLN | B | 84 | 26.975 | 2.750 | 24.186 | 1.00 | 28.25 | B |
| ATOM | 2106 | CA | GLN | B | 84 | 26.159 | 3.375 | 25.229 | 1.00 | 30.44 | B |
| ATOM | 2107 | CB | GLN | B | 84 | 25.467 | 2.310 | 26.093 | 1.00 | 34.30 | B |
| ATOM | 2108 | CG | GLN | B | 84 | 24.595 | 1.343 | 25.301 | 1.00 | 40.52 | B |
| ATOM | 2109 | CD | GLN | B | 84 | 23.515 | 2.047 | 24.496 | 1.00 | 43.21 | B |
| ATOM | 2110 | OE1 | GLN | B | 84 | 23.023 | 1.516 | 23.499 | 1.00 | 46.12 | B |
| ATOM | 2111 | NE2 | GLN | B | 84 | 23.133 | 3.244 | 24.932 | 1.00 | 45.41 | B |
| ATOM | 2112 | C | GLN | B | 84 | 27.030 | 4.254 | 26.111 | 1.00 | 29.01 | B |
| ATOM | 2113 | O | GLN | B | 84 | 26.633 | 5.353 | 26.494 | 1.00 | 27.82 | B |
| ATOM | 2114 | N | LEU | B | 85 | 28.219 | 3.757 | 26.436 | 1.00 | 28.32 | B |
| ATOM | 2115 | CA | LEU | B | 85 | 29.150 | 4.505 | 27.263 | 1.00 | 28.76 | B |
| ATOM | 2116 | CB | LEU | B | 85 | 30.355 | 3.631 | 27.631 | 1.00 | 28.92 | B |
| ATOM | 2117 | CG | LEU | B | 85 | 30.065 | 2.226 | 28.184 | 1.00 | 30.98 | B |
| ATOM | 2118 | CD1 | LEU | B | 85 | 31.343 | 1.631 | 28.758 | 1.00 | 30.59 | B |
| ATOM | 2119 | CD2 | LEU | B | 85 | 29.006 | 2.291 | 29.265 | 1.00 | 31.87 | B |
| ATOM | 2120 | C | LEU | B | 85 | 29.609 | 5.719 | 26.461 | 1.00 | 29.95 | B |
| ATOM | 2121 | O | LEU | B | 85 | 29.836 | 6.798 | 27.010 | 1.00 | 30.93 | B |
| ATOM | 2122 | N | GLU | B | 86 | 29.724 | 5.529 | 25.150 | 1.00 | 30.31 | B |
| ATOM | 2123 | CA | GLU | B | 86 | 30.160 | 6.577 | 24.245 | 1.00 | 31.41 | B |
| ATOM | 2124 | CB | GLU | B | 86 | 30.426 | 5.981 | 22.861 | 1.00 | 32.60 | B |
| ATOM | 2125 | CG | GLU | B | 86 | 31.741 | 6.420 | 22.236 | 1.00 | 39.25 | B |
| ATOM | 2126 | CD | GLU | B | 86 | 32.962 | 5.854 | 22.953 | 1.00 | 41.02 | B |
| ATOM | 2127 | OE1 | GLU | B | 86 | 33.379 | 4.714 | 22.636 | 1.00 | 40.75 | B |
| ATOM | 2128 | OE2 | GLU | B | 86 | 33.497 | 6.553 | 23.843 | 1.00 | 41.96 | B |
| ATOM | 2129 | C | GLU | B | 86 | 29.113 | 7.684 | 24.146 | 1.00 | 32.44 | B |
| ATOM | 2130 | O | GLU | B | 86 | 29.454 | 8.865 | 24.109 | 1.00 | 30.73 | B |
| ATOM | 2131 | N | LEU | B | 87 | 27.838 | 7.303 | 24.103 | 1.00 | 33.77 | B |
| ATOM | 2132 | CA | LEU | B | 87 | 26.755 | 8.282 | 24.015 | 1.00 | 34.65 | B |
| ATOM | 2133 | CB | LEU | B | 87 | 25.398 | 7.583 | 23.899 | 1.00 | 34.69 | B |
| ATOM | 2134 | CG | LEU | B | 87 | 24.916 | 7.169 | 22.508 | 1.00 | 36.86 | B |
| ATOM | 2135 | CD1 | LEU | B | 87 | 23.655 | 6.326 | 22.642 | 1.00 | 35.43 | B |
| ATOM | 2136 | CD2 | LEU | B | 87 | 24.645 | 8.411 | 21.660 | 1.00 | 35.76 | B |
| ATOM | 2137 | C | LEU | B | 87 | 26.740 | 9.199 | 25.231 | 1.00 | 35.16 | B |
| ATOM | 2138 | O | LEU | B | 87 | 26.250 | 10.326 | 25.164 | 1.00 | 34.29 | B |
| ATOM | 2139 | N | ARG | B | 88 | 27.280 | 8.711 | 26.343 | 1.00 | 36.69 | B |
| ATOM | 2140 | CA | ARG | B | 88 | 27.317 | 9.493 | 27.573 | 1.00 | 37.64 | B |
| ATOM | 2141 | CB | ARG | B | 88 | 27.173 | 8.575 | 28.791 | 1.00 | 39.79 | B |

| ATOM | 2142 | CG | ARG | B | 88 | 25.827 | 7.878 | 28.908 | 1.00 | 45.19 | B |
|------|------|-----|-----|---|----|--------|-------|--------|------|-------|---|
| ATOM | 2143 | CD | ARG | B | 88 | 25.704 | 7.173 | 30.253 | 1.00 | 49.04 | B |
| ATOM | 2144 | NE | ARG | B | 88 | 26.657 | 6.074 | 30.388 | 1.00 | 54.57 | B |
| ATOM | 2145 | CZ | ARG | B | 88 | 27.101 | 5.603 | 31.552 | 1.00 | 55.76 | B |
| ATOM | 2146 | NH1 | ARG | B | 88 | 26.683 | 6.137 | 32.694 | 1.00 | 55.56 | B |
| ATOM | 2147 | NH2 | ARG | B | 88 | 27.963 | 4.595 | 31.574 | 1.00 | 56.11 | B |
| ATOM | 2148 | C | ARG | B | 88 | 28.601 | 10.299 | 27.714 | 1.00 | 36.93 | B |
| ATOM | 2149 | O | ARG | B | 88 | 28.702 | 11.160 | 28.589 | 1.00 | 37.24 | B |
| ATOM | 2150 | N | THR | B | 89 | 29.571 | 10.035 | 26.842 | 1.00 | 35.19 | B |
| ATOM | 2151 | CA | THR | B | 89 | 30.860 | 10.712 | 26.914 | 1.00 | 31.71 | B |
| ATOM | 2152 | CB | THR | B | 89 | 31.916 | 9.767 | 27.529 | 1.00 | 31.61 | B |
| ATOM | 2153 | OG1 | THR | B | 89 | 31.980 | 8.554 | 26.762 | 1.00 | 29.72 | B |
| ATOM | 2154 | CG2 | THR | B | 89 | 31.557 | 9.436 | 28.963 | 1.00 | 25.87 | B |
| ATOM | 2155 | C | THR | B | 89 | 31.420 | 11.254 | 25.600 | 1.00 | 31.31 | B |
| ATOM | 2156 | O | THR | B | 89 | 31.214 | 12.415 | 25.249 | 1.00 | 32.41 | B |
| ATOM | 2157 | N | THR | B | 90 | 32.139 | 10.403 | 24.880 | 1.00 | 30.72 | B |
| ATOM | 2158 | CA | THR | B | 90 | 32.766 | 10.786 | 23.623 | 1.00 | 30.43 | B |
| ATOM | 2159 | CB | THR | B | 90 | 33.368 | 9.558 | 22.925 | 1.00 | 30.54 | B |
| ATOM | 2160 | OG1 | THR | B | 90 | 34.297 | 8.919 | 23.808 | 1.00 | 33.70 | B |
| ATOM | 2161 | CG2 | THR | B | 90 | 34.099 | 9.970 | 21.666 | 1.00 | 31.65 | B |
| ATOM | 2162 | C | THR | B | 90 | 31.874 | 11.512 | 22.625 | 1.00 | 30.61 | B |
| ATOM | 2163 | O | THR | B | 90 | 32.267 | 12.543 | 22.070 | 1.00 | 30.24 | B |
| ATOM | 2164 | N | LEU | B | 91 | 30.683 | 10.977 | 22.385 | 1.00 | 30.30 | B |
| ATOM | 2165 | CA | LEU | B | 91 | 29.767 | 11.581 | 21.425 | 1.00 | 31.93 | B |
| ATOM | 2166 | CB | LEU | B | 91 | 28.709 | 10.554 | 21.007 | 1.00 | 32.55 | B |
| ATOM | 2167 | CG | LEU | B | 91 | 29.268 | 9.315 | 20.292 | 1.00 | 33.01 | B |
| ATOM | 2168 | CD1 | LEU | B | 91 | 28.201 | 8.233 | 20.205 | 1.00 | 33.73 | B |
| ATOM | 2169 | CD2 | LEU | B | 91 | 29.761 | 9.700 | 18.902 | 1.00 | 31.26 | B |
| ATOM | 2170 | C | LEU | B | 91 | 29.096 | 12.872 | 21.907 | 1.00 | 32.38 | B |
| ATOM | 2171 | O | LEU | B | 91 | 28.402 | 13.534 | 21.139 | 1.00 | 32.08 | B |
| ATOM | 2172 | N | GLN | B | 92 | 29.303 | 13.229 | 23.173 | 1.00 | 32.44 | B |
| ATOM | 2173 | CA | GLN | B | 92 | 28.725 | 14.454 | 23.713 | 1.00 | 34.54 | B |
| ATOM | 2174 | CB | GLN | B | 92 | 28.138 | 14.217 | 25.110 | 1.00 | 38.48 | B |
| ATOM | 2175 | CG | GLN | B | 92 | 26.836 | 13.419 | 25.121 | 1.00 | 44.66 | B |
| ATOM | 2176 | CD | GLN | B | 92 | 26.233 | 13.291 | 26.516 | 1.00 | 49.27 | B |
| ATOM | 2177 | OE1 | GLN | B | 92 | 25.239 | 12.588 | 26.712 | 1.00 | 51.65 | B |
| ATOM | 2178 | NE2 | GLN | B | 92 | 26.832 | 13.975 | 27.491 | 1.00 | 49.93 | B |
| ATOM | 2179 | C | GLN | B | 92 | 29.779 | 15.557 | 23.777 | 1.00 | 32.86 | B |
| ATOM | 2180 | O | GLN | B | 92 | 29.457 | 16.721 | 24.019 | 1.00 | 32.19 | B |
| ATOM | 2181 | N | ARG | B | 93 | 31.038 | 15.187 | 23.555 | 1.00 | 31.53 | B |
| ATOM | 2182 | CA | ARG | B | 93 | 32.132 | 16.157 | 23.576 | 1.00 | 29.87 | B |
| ATOM | 2183 | CB | ARG | B | 93 | 33.477 | 15.472 | 23.302 | 1.00 | 28.14 | B |
| ATOM | 2184 | CG | ARG | B | 93 | 34.681 | 16.433 | 23.217 | 1.00 | 23.56 | B |
| ATOM | 2185 | CD | ARG | B | 93 | 35.953 | 15.656 | 22.925 | 1.00 | 22.53 | B |
| ATOM | 2186 | NE | ARG | B | 93 | 37.128 | 16.486 | 22.662 | 1.00 | 19.19 | B |
| ATOM | 2187 | CZ | ARG | B | 93 | 37.769 | 17.205 | 23.581 | 1.00 | 18.66 | B |
| ATOM | 2188 | NH1 | ARG | B | 93 | 37.352 | 17.214 | 24.843 | 1.00 | 17.45 | B |
| ATOM | 2189 | NH2 | ARG | B | 93 | 38.847 | 17.898 | 23.242 | 1.00 | 16.56 | B |
| ATOM | 2190 | C | ARG | B | 93 | 31.921 | 17.245 | 22.535 | 1.00 | 29.02 | B |
| ATOM | 2191 | O | ARG | B | 93 | 31.755 | 16.965 | 21.349 | 1.00 | 29.55 | B |
| ATOM | 2192 | N | ARG | B | 94 | 31.933 | 18.490 | 22.987 | 1.00 | 28.71 | B |
| ATOM | 2193 | CA | ARG | B | 94 | 31.767 | 19.613 | 22.087 | 1.00 | 29.63 | B |
| ATOM | 2194 | CB | ARG | B | 94 | 30.299 | 20.046 | 22.041 | 1.00 | 32.44 | B |
| ATOM | 2195 | CG | ARG | B | 94 | 29.506 | 19.196 | 21.060 | 1.00 | 37.10 | B |
| ATOM | 2196 | CD | ARG | B | 94 | 28.016 | 19.414 | 21.124 | 1.00 | 39.80 | B |
| ATOM | 2197 | NE | ARG | B | 94 | 27.350 | 18.742 | 20.008 | 1.00 | 44.04 | B |
| ATOM | 2198 | CZ | ARG | B | 94 | 27.372 | 17.428 | 19.791 | 1.00 | 44.11 | B |
| ATOM | 2199 | NH1 | ARG | B | 94 | 28.026 | 16.625 | 20.617 | 1.00 | 45.60 | B |
| ATOM | 2200 | NH2 | ARG | B | 94 | 26.747 | 16.916 | 18.739 | 1.00 | 44.45 | B |
| ATOM | 2201 | C | ARG | B | 94 | 32.656 | 20.760 | 22.498 | 1.00 | 28.84 | B |
| ATOM | 2202 | O | ARG | B | 94 | 32.464 | 21.363 | 23.550 | 1.00 | 29.13 | B |
| ATOM | 2203 | N | VAL | B | 95 | 33.650 | 21.038 | 21.663 | 1.00 | 27.49 | B |
| ATOM | 2204 | CA | VAL | B | 95 | 34.592 | 22.117 | 21.916 | 1.00 | 26.47 | B |
| ATOM | 2205 | CB | VAL | B | 95 | 36.047 | 21.605 | 21.890 | 1.00 | 25.65 | B |
| ATOM | 2206 | CG1 | VAL | B | 95 | 37.004 | 22.734 | 22.260 | 1.00 | 22.82 | B |
| ATOM | 2207 | CG2 | VAL | B | 95 | 36.202 | 20.423 | 22.849 | 1.00 | 26.01 | B |
| ATOM | 2208 | C | VAL | B | 95 | 34.415 | 23.180 | 20.840 | 1.00 | 27.00 | B |
| ATOM | 2209 | O | VAL | B | 95 | 34.721 | 22.945 | 19.665 | 1.00 | 27.00 | B |
| ATOM | 2210 | N | GLU | B | 96 | 33.912 | 24.340 | 21.253 | 1.00 | 26.94 | B |
| ATOM | 2211 | CA | GLU | B | 96 | 33.673 | 25.462 | 20.348 | 1.00 | 26.50 | B |
| ATOM | 2212 | CB | GLU | B | 96 | 33.072 | 26.649 | 21.107 | 1.00 | 29.19 | B |
| ATOM | 2213 | CG | GLU | B | 96 | 31.736 | 26.372 | 21.775 | 1.00 | 36.47 | B |
| ATOM | 2214 | CD | GLU | B | 96 | 31.211 | 27.582 | 22.537 | 1.00 | 40.45 | B |
| ATOM | 2215 | OE1 | GLU | B | 96 | 30.121 | 27.477 | 23.144 | 1.00 | 42.85 | B |

| ATOM | 2216 | OE2 | GLU | B | 96 | 31.891 | 28.634 | 22.526 | 1.00 | 40.11 | B |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2217 | C | GLU | B | 96 | 34.960 | 25.916 | 19.689 | 1.00 | 25.02 | B |
| ATOM | 2218 | O | GLU | B | 96 | 35.999 | 26.022 | 20.338 | 1.00 | 24.73 | B |
| ATOM | 2219 | N | PRO | B | 97 | 34.900 | 26.204 | 18.383 | 1.00 | 24.54 | B |
| ATOM | 2220 | CD | PRO | B | 97 | 33.744 | 26.011 | 17.493 | 1.00 | 22.89 | B |
| ATOM | 2221 | CA | PRO | B | 97 | 36.069 | 26.655 | 17.626 | 1.00 | 23.87 | B |
| ATOM | 2222 | CB | PRO | B | 97 | 35.580 | 26.633 | 16.175 | 1.00 | 22.81 | B |
| ATOM | 2223 | CG | PRO | B | 97 | 34.411 | 25.663 | 16.202 | 1.00 | 25.55 | B |
| ATOM | 2224 | C | PRO | B | 97 | 36.498 | 28.061 | 18.021 | 1.00 | 23.80 | B |
| ATOM | 2225 | O | PRO | B | 97 | 35.665 | 28.905 | 18.353 | 1.00 | 24.40 | B |
| ATOM | 2226 | N | THR | B | 98 | 37.799 | 28.307 | 17.990 | 1.00 | 22.02 | B |
| ATOM | 2227 | CA | THR | B | 98 | 38.306 | 29.634 | 18.266 | 1.00 | 24.00 | B |
| ATOM | 2228 | CB | THR | B | 98 | 39.569 | 29.592 | 19.150 | 1.00 | 27.31 | B |
| ATOM | 2229 | OG1 | THR | B | 98 | 40.626 | 28.929 | 18.449 | 1.00 | 35.69 | B |
| ATOM | 2230 | CG2 | THR | B | 98 | 39.282 | 28.839 | 20.439 | 1.00 | 26.76 | B |
| ATOM | 2231 | C | THR | B | 98 | 38.631 | 30.143 | 16.860 | 1.00 | 22.38 | B |
| ATOM | 2232 | O | THR | B | 98 | 39.376 | 29.504 | 16.116 | 1.00 | 19.48 | B |
| ATOM | 2233 | N | VAL | B | 99 | 38.041 | 31.274 | 16.487 | 1.00 | 21.55 | B |
| ATOM | 2234 | CA | VAL | B | 99 | 38.242 | 31.824 | 15.152 | 1.00 | 21.20 | B |
| ATOM | 2235 | CB | VAL | B | 99 | 36.871 | 32.153 | 14.509 | 1.00 | 21.09 | B |
| ATOM | 2236 | CG1 | VAL | B | 99 | 37.043 | 32.541 | 13.050 | 1.00 | 19.62 | B |
| ATOM | 2237 | CG2 | VAL | B | 99 | 35.950 | 30.944 | 14.625 | 1.00 | 18.29 | B |
| ATOM | 2238 | C | VAL | B | 99 | 39.140 | 33.059 | 15.167 | 1.00 | 21.59 | B |
| ATOM | 2239 | O | VAL | B | 99 | 38.970 | 33.962 | 15.982 | 1.00 | 21.57 | B |
| ATOM | 2240 | N | THR | B | 100 | 40.099 | 33.084 | 14.252 | 1.00 | 22.65 | B |
| ATOM | 2241 | CA | THR | B | 100 | 41.056 | 34.179 | 14.168 | 1.00 | 24.95 | B |
| ATOM | 2242 | CB | THR | B | 100 | 42.399 | 33.770 | 14.820 | 1.00 | 26.31 | B |
| ATOM | 2243 | OG1 | THR | B | 100 | 42.162 | 33.321 | 16.160 | 1.00 | 30.10 | B |
| ATOM | 2244 | CG2 | THR | B | 100 | 43.359 | 34.942 | 14.854 | 1.00 | 29.07 | B |
| ATOM | 2245 | C | THR | B | 100 | 41.329 | 34.556 | 12.717 | 1.00 | 24.61 | B |
| ATOM | 2246 | O | THR | B | 100 | 41.514 | 33.689 | 11.869 | 1.00 | 23.89 | B |
| ATOM | 2247 | N | ILE | B | 101 | 41.363 | 35.852 | 12.435 | 1.00 | 26.18 | B |
| ATOM | 2248 | CA | ILE | B | 101 | 41.638 | 36.315 | 11.080 | 1.00 | 29.32 | B |
| ATOM | 2249 | CB | ILE | B | 101 | 40.572 | 37.327 | 10.582 | 1.00 | 29.37 | B |
| ATOM | 2250 | CG2 | ILE | B | 101 | 40.986 | 37.885 | 9.231 | 1.00 | 29.49 | B |
| ATOM | 2251 | CG1 | ILE | B | 101 | 39.198 | 36.664 | 10.492 | 1.00 | 30.11 | B |
| ATOM | 2252 | CD1 | ILE | B | 101 | 38.110 | 37.605 | 10.002 | 1.00 | 29.81 | B |
| ATOM | 2253 | C | ILE | B | 101 | 42.988 | 37.015 | 11.040 | 1.00 | 31.04 | B |
| ATOM | 2254 | O | ILE | B | 101 | 43.270 | 37.868 | 11.877 | 1.00 | 31.24 | B |
| ATOM | 2255 | N | SER | B | 102 | 43.820 | 36.664 | 10.066 | 1.00 | 34.47 | B |
| ATOM | 2256 | CA | SER | B | 102 | 45.124 | 37.303 | 9.940 | 1.00 | 39.17 | B |
| ATOM | 2257 | CB | SER | B | 102 | 46.143 | 36.617 | 10.844 | 1.00 | 37.33 | B |
| ATOM | 2258 | OG | SER | B | 102 | 46.326 | 35.265 | 10.462 | 1.00 | 41.93 | B |
| ATOM | 2259 | C | SER | B | 102 | 45.632 | 37.289 | 8.501 | 1.00 | 42.45 | B |
| ATOM | 2260 | O | SER | B | 102 | 45.641 | 36.248 | 7.845 | 1.00 | 42.45 | B |
| ATOM | 2261 | N | PRO | B | 103 | 46.052 | 38.455 | 7.988 | 1.00 | 45.38 | B |
| ATOM | 2262 | CD | PRO | B | 103 | 45.938 | 39.793 | 8.596 | 1.00 | 45.47 | B |
| ATOM | 2263 | CA | PRO | B | 103 | 46.564 | 38.545 | 6.617 | 1.00 | 48.91 | B |
| ATOM | 2264 | CB | PRO | B | 103 | 46.446 | 40.032 | 6.312 | 1.00 | 47.74 | B |
| ATOM | 2265 | CG | PRO | B | 103 | 46.739 | 40.652 | 7.642 | 1.00 | 47.08 | B |
| ATOM | 2266 | C | PRO | B | 103 | 48.010 | 38.042 | 6.545 | 1.00 | 51.96 | B |
| ATOM | 2267 | O | PRO | B | 103 | 48.688 | 37.957 | 7.568 | 1.00 | 52.51 | B |
| ATOM | 2268 | N | SER | B | 104 | 48.475 | 37.699 | 5.346 | 1.00 | 55.84 | B |
| ATOM | 2269 | CA | SER | B | 104 | 49.843 | 37.209 | 5.177 | 1.00 | 60.00 | B |
| ATOM | 2270 | CB | SER | B | 104 | 50.018 | 36.578 | 3.791 | 1.00 | 59.60 | B |
| ATOM | 2271 | OG | SER | B | 104 | 49.778 | 37.520 | 2.759 | 1.00 | 59.05 | B |
| ATOM | 2272 | C | SER | B | 104 | 50.842 | 38.353 | 5.368 | 1.00 | 63.75 | B |
| ATOM | 2273 | O | SER | B | 104 | 50.853 | 39.325 | 4.605 | 1.00 | 64.64 | B |
| ATOM | 2274 | N | ARG | B | 105 | 51.677 | 38.228 | 6.398 | 1.00 | 66.99 | B |
| ATOM | 2275 | CA | ARG | B | 105 | 52.674 | 39.242 | 6.736 | 1.00 | 69.17 | B |
| ATOM | 2276 | CB | ARG | B | 105 | 53.631 | 38.700 | 7.808 | 1.00 | 70.33 | B |
| ATOM | 2277 | CG | ARG | B | 105 | 54.672 | 37.690 | 7.318 | 1.00 | 72.24 | B |
| ATOM | 2278 | CD | ARG | B | 105 | 54.073 | 36.586 | 6.449 | 1.00 | 73.51 | B |
| ATOM | 2279 | NE | ARG | B | 105 | 52.981 | 35.859 | 7.095 | 1.00 | 75.02 | B |
| ATOM | 2280 | CZ | ARG | B | 105 | 53.120 | 35.051 | 8.142 | 1.00 | 76.07 | B |
| ATOM | 2281 | NH1 | ARG | B | 105 | 54.314 | 34.852 | 8.684 | 1.00 | 77.38 | B |
| ATOM | 2282 | NH2 | ARG | B | 105 | 52.059 | 34.431 | 8.644 | 1.00 | 76.05 | B |
| ATOM | 2283 | C | ARG | B | 105 | 53.464 | 39.720 | 5.523 | 1.00 | 70.38 | B |
| ATOM | 2284 | O | ARG | B | 105 | 53.134 | 40.746 | 4.923 | 1.00 | 71.56 | B |
| ATOM | 2285 | N | ASN | B | 113 | 46.629 | 40.478 | -1.867 | 1.00 | 49.25 | B |
| ATOM | 2286 | CA | ASN | B | 113 | 46.963 | 40.039 | -0.515 | 1.00 | 48.42 | B |
| ATOM | 2287 | CB | ASN | B | 113 | 46.726 | 41.181 | 0.477 | 1.00 | 51.23 | B |
| ATOM | 2288 | CG | ASN | B | 113 | 47.268 | 40.875 | 1.863 | 1.00 | 53.89 | B |
| ATOM | 2289 | OD1 | ASN | B | 113 | 48.429 | 40.498 | 2.019 | 1.00 | 55.14 | B |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2290 | ND2 | ASN | B | 113 | 46.428 | 41.048 | 2.880 | 1.00 | 55.30 | B |
| ATOM | 2291 | C | ASN | B | 113 | 46.143 | 38.808 | -0.118 | 1.00 | 45.78 | B |
| ATOM | 2292 | O | ASN | B | 113 | 45.155 | 38.471 | -0.774 | 1.00 | 44.99 | B |
| ATOM | 2293 | N | LEU | B | 114 | 46.550 | 38.146 | 0.961 | 1.00 | 42.27 | B |
| ATOM | 2294 | CA | LEU | B | 114 | 45.862 | 36.944 | 1.415 | 1.00 | 38.77 | B |
| ATOM | 2295 | CB | LEU | B | 114 | 46.770 | 35.739 | 1.182 | 1.00 | 39.10 | B |
| ATOM | 2296 | CG | LEU | B | 114 | 46.238 | 34.330 | 1.421 | 1.00 | 40.81 | B |
| ATOM | 2297 | CD1 | LEU | B | 114 | 45.097 | 34.023 | 0.459 | 1.00 | 41.59 | B |
| ATOM | 2298 | CD2 | LEU | B | 114 | 47.379 | 33.341 | 1.222 | 1.00 | 41.03 | B |
| ATOM | 2299 | C | LEU | B | 114 | 45.424 | 36.986 | 2.883 | 1.00 | 36.39 | B |
| ATOM | 2300 | O | LEU | B | 114 | 46.237 | 37.204 | 3.783 | 1.00 | 35.98 | B |
| ATOM | 2301 | N | LEU | B | 115 | 44.130 | 36.777 | 3.112 | 1.00 | 31.79 | B |
| ATOM | 2302 | CA | LEU | B | 115 | 43.576 | 36.766 | 4.460 | 1.00 | 28.77 | B |
| ATOM | 2303 | CB | LEU | B | 115 | 42.231 | 37.496 | 4.493 | 1.00 | 29.52 | B |
| ATOM | 2304 | CG | LEU | B | 115 | 42.156 | 38.843 | 5.218 | 1.00 | 30.12 | B |
| ATOM | 2305 | CD1 | LEU | B | 115 | 43.281 | 39.751 | 4.764 | 1.00 | 30.28 | B |
| ATOM | 2306 | CD2 | LEU | B | 115 | 40.799 | 39.479 | 4.951 | 1.00 | 28.39 | B |
| ATOM | 2307 | C | LEU | B | 115 | 43.374 | 35.323 | 4.896 | 1.00 | 27.23 | B |
| ATOM | 2308 | O | LEU | B | 115 | 42.815 | 34.513 | 4.154 | 1.00 | 25.72 | B |
| ATOM | 2309 | N | VAL | B | 116 | 43.825 | 35.002 | 6.103 | 1.00 | 24.13 | B |
| ATOM | 2310 | CA | VAL | B | 116 | 43.695 | 33.651 | 6.618 | 1.00 | 20.76 | B |
| ATOM | 2311 | CB | VAL | B | 116 | 45.078 | 33.098 | 7.078 | 1.00 | 20.02 | B |
| ATOM | 2312 | CG1 | VAL | B | 116 | 44.915 | 31.757 | 7.777 | 1.00 | 17.46 | B |
| ATOM | 2313 | CG2 | VAL | B | 116 | 45.996 | 32.944 | 5.880 | 1.00 | 19.44 | B |
| ATOM | 2314 | C | VAL | B | 116 | 42.723 | 33.568 | 7.784 | 1.00 | 20.38 | B |
| ATOM | 2315 | O | VAL | B | 116 | 42.860 | 34.293 | 8.766 | 1.00 | 19.54 | B |
| ATOM | 2316 | N | CYS | B | 117 | 41.724 | 32.701 | 7.669 | 1.00 | 20.87 | B |
| ATOM | 2317 | CA | CYS | B | 117 | 40.793 | 32.523 | 8.774 | 1.00 | 22.57 | B |
| ATOM | 2318 | C | CYS | B | 117 | 41.132 | 31.196 | 9.444 | 1.00 | 21.84 | B |
| ATOM | 2319 | O | CYS | B | 117 | 40.867 | 30.123 | 8.892 | 1.00 | 22.98 | B |
| ATOM | 2320 | CB | CYS | B | 117 | 39.332 | 32.486 | 8.315 | 1.00 | 23.53 | B |
| ATOM | 2321 | SG | CYS | B | 117 | 38.217 | 32.222 | 9.734 | 1.00 | 29.76 | B |
| ATOM | 2322 | N | SER | B | 118 | 41.728 | 31.277 | 10.627 | 1.00 | 19.87 | B |
| ATOM | 2323 | CA | SER | B | 118 | 42.094 | 30.092 | 11.381 | 1.00 | 18.65 | B |
| ATOM | 2324 | CB | SER | B | 118 | 43.345 | 30.356 | 12.226 | 1.00 | 19.67 | B |
| ATOM | 2325 | OG | SER | B | 118 | 44.463 | 30.672 | 11.421 | 1.00 | 22.97 | B |
| ATOM | 2326 | C | SER | B | 118 | 40.962 | 29.656 | 12.300 | 1.00 | 18.03 | B |
| ATOM | 2327 | O | SER | B | 118 | 40.579 | 30.389 | 13.209 | 1.00 | 19.82 | B |
| ATOM | 2328 | N | VAL | B | 119 | 40.426 | 28.463 | 12.050 | 1.00 | 17.57 | B |
| ATOM | 2329 | CA | VAL | B | 119 | 39.365 | 27.889 | 12.874 | 1.00 | 15.30 | B |
| ATOM | 2330 | CB | VAL | B | 119 | 38.202 | 27.364 | 12.006 | 1.00 | 15.69 | B |
| ATOM | 2331 | CG1 | VAL | B | 119 | 37.091 | 26.852 | 12.892 | 1.00 | 11.64 | B |
| ATOM | 2332 | CG2 | VAL | B | 119 | 37.695 | 28.484 | 11.076 | 1.00 | 13.82 | B |
| ATOM | 2333 | C | VAL | B | 119 | 40.073 | 26.739 | 13.579 | 1.00 | 15.38 | B |
| ATOM | 2334 | O | VAL | B | 119 | 40.318 | 25.680 | 12.992 | 1.00 | 16.76 | B |
| ATOM | 2335 | N | THR | B | 120 | 40.404 | 26.958 | 14.844 | 1.00 | 16.03 | B |
| ATOM | 2336 | CA | THR | B | 120 | 41.165 | 25.988 | 15.615 | 1.00 | 15.04 | B |
| ATOM | 2337 | CB | THR | B | 120 | 42.487 | 26.613 | 16.031 | 1.00 | 13.75 | B |
| ATOM | 2338 | OG1 | THR | B | 120 | 42.221 | 27.713 | 16.915 | 1.00 | 17.84 | B |
| ATOM | 2339 | CG2 | THR | B | 120 | 43.230 | 27.144 | 14.815 | 1.00 | 12.18 | B |
| ATOM | 2340 | C | THR | B | 120 | 40.533 | 25.405 | 16.872 | 1.00 | 17.87 | B |
| ATOM | 2341 | O | THR | B | 120 | 39.571 | 25.944 | 17.425 | 1.00 | 17.71 | B |
| ATOM | 2342 | N | ASP | B | 121 | 41.132 | 24.303 | 17.317 | 1.00 | 19.07 | B |
| ATOM | 2343 | CA | ASP | B | 121 | 40.738 | 23.576 | 18.511 | 1.00 | 20.97 | B |
| ATOM | 2344 | CB | ASP | B | 121 | 41.268 | 24.291 | 19.766 | 1.00 | 24.82 | B |
| ATOM | 2345 | CG | ASP | B | 121 | 42.797 | 24.330 | 19.831 | 1.00 | 31.04 | B |
| ATOM | 2346 | OD1 | ASP | B | 121 | 43.460 | 23.360 | 19.397 | 1.00 | 30.81 | B |
| ATOM | 2347 | OD2 | ASP | B | 121 | 43.339 | 25.333 | 20.346 | 1.00 | 34.38 | B |
| ATOM | 2348 | C | ASP | B | 121 | 39.238 | 23.293 | 18.679 | 1.00 | 21.27 | B |
| ATOM | 2349 | O | ASP | B | 121 | 38.629 | 23.671 | 19.683 | 1.00 | 23.00 | B |
| ATOM | 2350 | N | PHE | B | 122 | 38.641 | 22.613 | 17.710 | 1.00 | 20.38 | B |
| ATOM | 2351 | CA | PHE | B | 122 | 37.233 | 22.280 | 17.818 | 1.00 | 18.51 | B |
| ATOM | 2352 | CB | PHE | B | 122 | 36.414 | 22.988 | 16.732 | 1.00 | 16.18 | B |
| ATOM | 2353 | CG | PHE | B | 122 | 36.817 | 22.644 | 15.319 | 1.00 | 13.31 | B |
| ATOM | 2354 | CD1 | PHE | B | 122 | 37.695 | 23.463 | 14.615 | 1.00 | 11.43 | B |
| ATOM | 2355 | CD2 | PHE | B | 122 | 36.247 | 21.547 | 14.664 | 1.00 | 10.93 | B |
| ATOM | 2356 | CE1 | PHE | B | 122 | 37.998 | 23.210 | 13.272 | 1.00 | 10.91 | B |
| ATOM | 2357 | CE2 | PHE | B | 122 | 36.541 | 21.280 | 13.317 | 1.00 | 12.31 | B |
| ATOM | 2358 | CZ | PHE | B | 122 | 37.419 | 22.118 | 12.618 | 1.00 | 8.92 | B |
| ATOM | 2359 | C | PHE | B | 122 | 37.011 | 20.778 | 17.739 | 1.00 | 19.55 | B |
| ATOM | 2360 | O | PHE | B | 122 | 37.889 | 20.029 | 17.301 | 1.00 | 18.45 | B |
| ATOM | 2361 | N | TYR | B | 123 | 35.829 | 20.357 | 18.182 | 1.00 | 20.50 | B |
| ATOM | 2362 | CA | TYR | B | 123 | 35.412 | 18.959 | 18.180 | 1.00 | 21.08 | B |
| ATOM | 2363 | CB | TYR | B | 123 | 36.067 | 18.201 | 19.340 | 1.00 | 19.11 | B |

| ATOM | 2364 | CG | TYR | B | 123 | 35.919 | 16.702 | 19.228 | 1.00 | 18.56 | B |
|------|------|------|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2365 | CD1 | TYR | B | 123 | 34.746 | 16.062 | 19.629 | 1.00 | 19.13 | B |
| ATOM | 2366 | CE1 | TYR | B | 123 | 34.572 | 14.695 | 19.446 | 1.00 | 17.75 | B |
| ATOM | 2367 | CD2 | TYR | B | 123 | 36.920 | 15.932 | 18.647 | 1.00 | 17.20 | B |
| ATOM | 2368 | CE2 | TYR | B | 123 | 36.762 | 14.566 | 18.455 | 1.00 | 17.38 | B |
| ATOM | 2369 | CZ | TYR | B | 123 | 35.584 | 13.953 | 18.853 | 1.00 | 19.59 | B |
| ATOM | 2370 | OH | TYR | B | 123 | 35.412 | 12.608 | 18.631 | 1.00 | 22.32 | B |
| ATOM | 2371 | C | TYR | B | 123 | 33.896 | 18.957 | 18.351 | 1.00 | 21.83 | B |
| ATOM | 2372 | O | TYR | B | 123 | 33.365 | 19.708 | 19.165 | 1.00 | 23.26 | B |
| ATOM | 2373 | N | PRO | B | 124 | 33.175 | 18.126 | 17.584 | 1.00 | 21.65 | B |
| ATOM | 2374 | CD | PRO | B | 124 | 31.725 | 17.996 | 17.808 | 1.00 | 23.81 | B |
| ATOM | 2375 | CA | PRO | B | 124 | 33.627 | 17.177 | 16.562 | 1.00 | 22.30 | B |
| ATOM | 2376 | CB | PRO | B | 124 | 32.398 | 16.290 | 16.353 | 1.00 | 21.95 | B |
| ATOM | 2377 | CG | PRO | B | 124 | 31.270 | 17.237 | 16.586 | 1.00 | 23.07 | B |
| ATOM | 2378 | C | PRO | B | 124 | 34.128 | 17.813 | 15.266 | 1.00 | 22.20 | B |
| ATOM | 2379 | O | PRO | B | 124 | 34.204 | 19.035 | 15.149 | 1.00 | 24.43 | B |
| ATOM | 2380 | N | ALA | B | 125 | 34.457 | 16.971 | 14.291 | 1.00 | 20.63 | B |
| ATOM | 2381 | CA | ALA | B | 125 | 34.987 | 17.428 | 13.007 | 1.00 | 22.13 | B |
| ATOM | 2382 | CB | ALA | B | 125 | 35.571 | 16.236 | 12.244 | 1.00 | 20.20 | B |
| ATOM | 2383 | C | ALA | B | 125 | 34.057 | 18.222 | 12.078 | 1.00 | 22.42 | B |
| ATOM | 2384 | O | ALA | B | 125 | 34.512 | 19.129 | 11.400 | 1.00 | 24.48 | B |
| ATOM | 2385 | N | GLN | B | 126 | 32.772 | 17.893 | 12.036 | 1.00 | 25.59 | B |
| ATOM | 2386 | CA | GLN | B | 126 | 31.845 | 18.598 | 11.147 | 1.00 | 27.46 | B |
| ATOM | 2387 | CB | GLN | B | 126 | 30.414 | 18.101 | 11.357 | 1.00 | 29.99 | B |
| ATOM | 2388 | CG | GLN | B | 126 | 30.283 | 16.595 | 11.480 | 1.00 | 36.21 | B |
| ATOM | 2389 | CD | GLN | B | 126 | 30.625 | 16.102 | 12.870 | 1.00 | 38.28 | B |
| ATOM | 2390 | OE1 | GLN | B | 126 | 30.558 | 14.905 | 13.158 | 1.00 | 40.46 | B |
| ATOM | 2391 | NE2 | GLN | B | 126 | 30.989 | 17.030 | 13.745 | 1.00 | 40.92 | B |
| ATOM | 2392 | C | GLN | B | 126 | 31.876 | 20.112 | 11.333 | 1.00 | 28.28 | B |
| ATOM | 2393 | O | GLN | B | 126 | 31.571 | 20.627 | 12.410 | 1.00 | 29.36 | B |
| ATOM | 2394 | N | ILE | B | 127 | 32.221 | 20.831 | 10.273 | 1.00 | 27.17 | B |
| ATOM | 2395 | CA | ILE | B | 127 | 32.292 | 22.279 | 10.353 | 1.00 | 27.02 | B |
| ATOM | 2396 | CB | ILE | B | 127 | 33.656 | 22.716 | 10.931 | 1.00 | 27.21 | B |
| ATOM | 2397 | CG2 | ILE | B | 127 | 34.767 | 22.453 | 9.898 | 1.00 | 21.63 | B |
| ATOM | 2398 | CG1 | ILE | B | 127 | 33.612 | 24.195 | 11.316 | 1.00 | 24.63 | B |
| ATOM | 2399 | CD1 | ILE | B | 127 | 34.760 | 24.633 | 12.198 | 1.00 | 25.86 | B |
| ATOM | 2400 | C | ILE | B | 127 | 32.117 | 22.903 | 8.969 | 1.00 | 27.10 | B |
| ATOM | 2401 | O | ILE | B | 127 | 32.393 | 22.258 | 7.956 | 1.00 | 26.58 | B |
| ATOM | 2402 | N | LYS | B | 128 | 31.666 | 24.155 | 8.940 | 1.00 | 25.41 | B |
| ATOM | 2403 | CA | LYS | B | 128 | 31.457 | 24.884 | 7.689 | 1.00 | 27.45 | B |
| ATOM | 2404 | CB | LYS | B | 128 | 29.964 | 24.927 | 7.334 | 1.00 | 29.68 | B |
| ATOM | 2405 | CG | LYS | B | 128 | 29.633 | 25.685 | 6.046 | 1.00 | 34.69 | B |
| ATOM | 2406 | CD | LYS | B | 128 | 30.129 | 24.954 | 4.793 | 1.00 | 38.25 | B |
| ATOM | 2407 | CE | LYS | B | 128 | 29.802 | 25.742 | 3.517 | 1.00 | 40.20 | B |
| ATOM | 2408 | NZ | LYS | B | 128 | 30.281 | 25.071 | 2.271 | 1.00 | 39.87 | B |
| ATOM | 2409 | C | LYS | B | 128 | 31.983 | 26.301 | 7.861 | 1.00 | 25.41 | B |
| ATOM | 2410 | O | LYS | B | 128 | 31.559 | 27.019 | 8.759 | 1.00 | 26.68 | B |
| ATOM | 2411 | N | VAL | B | 129 | 32.911 | 26.700 | 7.002 | 1.00 | 25.70 | B |
| ATOM | 2412 | CA | VAL | B | 129 | 33.493 | 28.034 | 7.078 | 1.00 | 24.82 | B |
| ATOM | 2413 | CB | VAL | B | 129 | 35.013 | 27.956 | 7.329 | 1.00 | 24.17 | B |
| ATOM | 2414 | CG1 | VAL | B | 129 | 35.592 | 29.351 | 7.452 | 1.00 | 22.14 | B |
| ATOM | 2415 | CG2 | VAL | B | 129 | 35.295 | 27.136 | 8.583 | 1.00 | 22.44 | B |
| ATOM | 2416 | C | VAL | B | 129 | 33.248 | 28.791 | 5.778 | 1.00 | 25.17 | B |
| ATOM | 2417 | O | VAL | B | 129 | 33.532 | 28.283 | 4.701 | 1.00 | 25.50 | B |
| ATOM | 2418 | N | ARG | B | 130 | 32.724 | 30.007 | 5.884 | 1.00 | 27.21 | B |
| ATOM | 2419 | CA | ARG | B | 130 | 32.445 | 30.814 | 4.701 | 1.00 | 28.49 | B |
| ATOM | 2420 | CB | ARG | B | 130 | 30.931 | 30.920 | 4.470 | 1.00 | 31.77 | B |
| ATOM | 2421 | CG | ARG | B | 130 | 30.239 | 29.591 | 4.183 | 1.00 | 34.92 | B |
| ATOM | 2422 | CD | ARG | B | 130 | 28.927 | 29.813 | 3.432 | 1.00 | 41.30 | B |
| ATOM | 2423 | NE | ARG | B | 130 | 27.834 | 30.254 | 4.291 | 1.00 | 42.15 | B |
| ATOM | 2424 | CZ | ARG | B | 130 | 27.032 | 29.426 | 4.953 | 1.00 | 46.05 | B |
| ATOM | 2425 | NH1 | ARG | B | 130 | 27.200 | 28.112 | 4.849 | 1.00 | 45.50 | B |
| ATOM | 2426 | NH2 | ARG | B | 130 | 26.061 | 29.910 | 5.718 | 1.00 | 48.30 | B |
| ATOM | 2427 | C | ARG | B | 130 | 33.036 | 32.211 | 4.792 | 1.00 | 27.57 | B |
| ATOM | 2428 | O | ARG | B | 130 | 33.130 | 32.789 | 5.874 | 1.00 | 26.00 | B |
| ATOM | 2429 | N | TRP | B | 131 | 33.440 | 32.744 | 3.645 | 1.00 | 27.37 | B |
| ATOM | 2430 | CA | TRP | B | 131 | 34.004 | 34.085 | 3.571 | 1.00 | 30.27 | B |
| ATOM | 2431 | CB | TRP | B | 131 | 35.281 | 34.083 | 2.737 | 1.00 | 30.21 | B |
| ATOM | 2432 | CG | TRP | B | 131 | 36.532 | 33.844 | 3.521 | 1.00 | 32.32 | B |
| ATOM | 2433 | CD2 | TRP | B | 131 | 37.155 | 34.757 | 4.432 | 1.00 | 32.41 | B |
| ATOM | 2434 | CE2 | TRP | B | 131 | 38.334 | 34.142 | 4.900 | 1.00 | 33.07 | B |
| ATOM | 2435 | CE3 | TRP | B | 131 | 36.831 | 36.039 | 4.897 | 1.00 | 31.75 | B |
| ATOM | 2436 | CD1 | TRP | B | 131 | 37.333 | 32.741 | 3.478 | 1.00 | 32.80 | B |
| ATOM | 2437 | NE1 | TRP | B | 131 | 38.420 | 32.913 | 4.300 | 1.00 | 31.53 | B |

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ATOM   2438  CZ2 TRP B 131      39.193  34.764   5.812  1.00 32.82      B
ATOM   2439  CZ3 TRP B 131      37.680  36.656   5.800  1.00 32.08      B
ATOM   2440  CH2 TRP B 131      38.849  36.017   6.249  1.00 33.40      B
ATOM   2441  C   TRP B 131      33.003  35.064   2.949  1.00 32.99      B
ATOM   2442  O   TRP B 131      32.367  34.759   1.940  1.00 32.18      B
ATOM   2443  N   PHE B 132      32.879  36.242   3.550  1.00 35.48      B
ATOM   2444  CA  PHE B 132      31.962  37.263   3.058  1.00 39.35      B
ATOM   2445  CB  PHE B 132      30.856  37.501   4.077  1.00 38.14      B
ATOM   2446  CG  PHE B 132      29.843  36.407   4.123  1.00 38.39      B
ATOM   2447  CD1 PHE B 132      28.804  36.373   3.202  1.00 38.31      B
ATOM   2448  CD2 PHE B 132      29.930  35.399   5.075  1.00 38.21      B
ATOM   2449  CE1 PHE B 132      27.860  35.348   3.229  1.00 39.26      B
ATOM   2450  CE2 PHE B 132      28.992  34.369   5.111  1.00 38.83      B
ATOM   2451  CZ  PHE B 132      27.954  34.345   4.184  1.00 37.91      B
ATOM   2452  C   PHE B 132      32.650  38.583   2.755  1.00 41.59      B
ATOM   2453  O   PHE B 132      33.515  39.025   3.508  1.00 42.72      B
ATOM   2454  N   ARG B 133      32.267  39.203   1.640  1.00 45.04      B
ATOM   2455  CA  ARG B 133      32.829  40.490   1.242  1.00 48.28      B
ATOM   2456  CB  ARG B 133      32.510  40.787  -0.227  1.00 51.68      B
ATOM   2457  CG  ARG B 133      33.293  41.958  -0.829  1.00 55.78      B
ATOM   2458  CD  ARG B 133      34.787  41.655  -0.867  1.00 57.07      B
ATOM   2459  NE  ARG B 133      35.580  42.741  -1.440  1.00 59.30      B
ATOM   2460  CZ  ARG B 133      35.523  43.135  -2.710  1.00 60.93      B
ATOM   2461  NH1 ARG B 133      34.702  42.536  -3.564  1.00 61.44      B
ATOM   2462  NH2 ARG B 133      36.295  44.132  -3.128  1.00 61.77      B
ATOM   2463  C   ARG B 133      32.129  41.492   2.145  1.00 49.07      B
ATOM   2464  O   ARG B 133      32.299  41.460   3.358  1.00 51.26      B
ATOM   2465  N   ASN B 134      31.331  42.376   1.572  1.00 49.23      B
ATOM   2466  CA  ASN B 134      30.614  43.336   2.393  1.00 48.83      B
ATOM   2467  CB  ASN B 134      30.582  44.702   1.710  1.00 45.93      B
ATOM   2468  CG  ASN B 134      31.973  45.290   1.523  1.00 45.10      B
ATOM   2469  OD1 ASN B 134      32.450  45.440   0.397  1.00 41.81      B
ATOM   2470  ND2 ASN B 134      32.634  45.618   2.634  1.00 41.82      B
ATOM   2471  C   ASN B 134      29.203  42.795   2.594  1.00 50.25      B
ATOM   2472  O   ASN B 134      28.222  43.529   2.508  1.00 52.28      B
ATOM   2473  N   ASP B 135      29.122  41.496   2.868  1.00 50.15      B
ATOM   2474  CA  ASP B 135      27.847  40.819   3.072  1.00 51.07      B
ATOM   2475  C   ASP B 135      27.590  39.855   1.910  1.00 51.76      B
ATOM   2476  O   ASP B 135      26.586  39.136   1.893  1.00 51.82      B
ATOM   2477  N   GLN B 136      28.507  39.856   0.944  1.00 50.97      B
ATOM   2478  CA  GLN B 136      28.421  38.999  -0.240  1.00 51.24      B
ATOM   2479  CB  GLN B 136      28.766  39.805  -1.493  1.00 53.78      B
ATOM   2480  CG  GLN B 136      28.736  39.000  -2.783  1.00 58.16      B
ATOM   2481  CD  GLN B 136      29.675  39.559  -3.839  1.00 59.39      B
ATOM   2482  OE1 GLN B 136      30.895  39.527  -3.675  1.00 60.12      B
ATOM   2483  NE2 GLN B 136      29.110  40.078  -4.926  1.00 59.45      B
ATOM   2484  C   GLN B 136      29.395  37.825  -0.124  1.00 49.46      B
ATOM   2485  O   GLN B 136      30.607  38.026  -0.035  1.00 48.29      B
ATOM   2486  N   GLU B 137      28.873  36.603  -0.144  1.00 47.64      B
ATOM   2487  CA  GLU B 137      29.730  35.432  -0.027  1.00 46.85      B
ATOM   2488  CB  GLU B 137      28.899  34.152   0.022  1.00 47.17      B
ATOM   2489  CG  GLU B 137      29.695  32.975   0.556  1.00 50.22      B
ATOM   2490  CD  GLU B 137      28.866  31.726   0.743  1.00 52.65      B
ATOM   2491  OE1 GLU B 137      27.699  31.842   1.171  1.00 55.57      B
ATOM   2492  OE2 GLU B 137      29.391  30.623   0.478  1.00 54.41      B
ATOM   2493  C   GLU B 137      30.755  35.320  -1.149  1.00 45.23      B
ATOM   2494  O   GLU B 137      30.445  35.544  -2.314  1.00 45.04      B
ATOM   2495  N   GLU B 138      31.983  34.977  -0.776  1.00 44.63      B
ATOM   2496  CA  GLU B 138      33.078  34.808  -1.724  1.00 44.36      B
ATOM   2497  CB  GLU B 138      34.284  35.658  -1.307  1.00 45.65      B
ATOM   2498  CG  GLU B 138      34.076  37.166  -1.320  1.00 48.42      B
ATOM   2499  CD  GLU B 138      34.144  37.761  -2.717  1.00 50.71      B
ATOM   2500  OE1 GLU B 138      35.120  37.471  -3.442  1.00 51.60      B
ATOM   2501  OE2 GLU B 138      33.227  38.526  -3.086  1.00 50.99      B
ATOM   2502  C   GLU B 138      33.498  33.335  -1.740  1.00 43.68      B
ATOM   2503  O   GLU B 138      33.831  32.769  -0.697  1.00 43.53      B
ATOM   2504  N   THR B 139      33.468  32.711  -2.914  1.00 42.58      B
ATOM   2505  CA  THR B 139      33.881  31.313  -3.044  1.00 41.76      B
ATOM   2506  CB  THR B 139      32.739  30.415  -3.543  1.00 41.04      B
ATOM   2507  OG1 THR B 139      32.207  30.948  -4.759  1.00 40.71      B
ATOM   2508  CG2 THR B 139      31.641  30.325  -2.492  1.00 41.89      B
ATOM   2509  C   THR B 139      35.038  31.245  -4.026  1.00 40.93      B
ATOM   2510  O   THR B 139      35.855  30.326  -3.981  1.00 40.04      B
ATOM   2511  N   ALA B 140      35.096  32.224  -4.920  1.00 40.67      B
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ATOM    2512   CA   ALA B 140      36.179   32.305   -5.887   1.00  41.22      B
ATOM    2513   CB   ALA B 140      35.714   33.016   -7.158   1.00  41.13      B
ATOM    2514   C    ALA B 140      37.247   33.126   -5.177   1.00  41.09      B
ATOM    2515   O    ALA B 140      36.976   34.232   -4.693   1.00  43.11      B
ATOM    2516   N    GLY B 141      38.455   32.582   -5.102   1.00  39.60      B
ATOM    2517   CA   GLY B 141      39.526   33.278   -4.418   1.00  35.11      B
ATOM    2518   C    GLY B 141      39.739   32.651   -3.051   1.00  33.42      B
ATOM    2519   O    GLY B 141      40.605   33.076   -2.287   1.00  31.24      B
ATOM    2520   N    VAL B 142      38.945   31.628   -2.750   1.00  31.89      B
ATOM    2521   CA   VAL B 142      39.033   30.937   -1.470   1.00  32.27      B
ATOM    2522   CB   VAL B 142      37.645   30.790   -0.813   1.00  31.90      B
ATOM    2523   CG1  VAL B 142      37.733   29.861    0.400   1.00  32.37      B
ATOM    2524   CG2  VAL B 142      37.125   32.161   -0.402   1.00  32.53      B
ATOM    2525   C    VAL B 142      39.652   29.552   -1.564   1.00  31.26      B
ATOM    2526   O    VAL B 142      39.211   28.712   -2.343   1.00  32.44      B
ATOM    2527   N    VAL B 143      40.676   29.326   -0.752   1.00  30.76      B
ATOM    2528   CA   VAL B 143      41.357   28.045   -0.702   1.00  29.79      B
ATOM    2529   CB   VAL B 143      42.815   28.154   -1.162   1.00  29.63      B
ATOM    2530   CG1  VAL B 143      43.439   26.768   -1.212   1.00  31.60      B
ATOM    2531   CG2  VAL B 143      42.885   28.819   -2.514   1.00  33.43      B
ATOM    2532   C    VAL B 143      41.357   27.575    0.749   1.00  30.61      B
ATOM    2533   O    VAL B 143      41.665   28.338    1.667   1.00  28.64      B
ATOM    2534   N    SER B 144      41.017   26.313    0.950   1.00  29.65      B
ATOM    2535   CA   SER B 144      40.970   25.756    2.282   1.00  28.42      B
ATOM    2536   CB   SER B 144      39.541   25.325    2.605   1.00  29.23      B
ATOM    2537   OG   SER B 144      39.457   24.705    3.875   1.00  33.81      B
ATOM    2538   C    SER B 144      41.900   24.562    2.373   1.00  27.32      B
ATOM    2539   O    SER B 144      42.101   23.840    1.397   1.00  27.40      B
ATOM    2540   N    THR B 145      42.492   24.372    3.542   1.00  25.70      B
ATOM    2541   CA   THR B 145      43.364   23.227    3.755   1.00  24.82      B
ATOM    2542   CB   THR B 145      44.272   23.418    4.995   1.00  25.01      B
ATOM    2543   OG1  THR B 145      43.467   23.399    6.186   1.00  25.18      B
ATOM    2544   CG2  THR B 145      45.022   24.743    4.923   1.00  23.27      B
ATOM    2545   C    THR B 145      42.392   22.100    4.071   1.00  24.16      B
ATOM    2546   O    THR B 145      41.200   22.335    4.272   1.00  23.86      B
ATOM    2547   N    PRO B 146      42.865   20.854    4.081   1.00  23.17      B
ATOM    2548   CD   PRO B 146      44.116   20.231    3.618   1.00  22.29      B
ATOM    2549   CA   PRO B 146      41.854   19.852    4.419   1.00  23.18      B
ATOM    2550   CB   PRO B 146      42.521   18.536    4.008   1.00  24.20      B
ATOM    2551   CG   PRO B 146      43.998   18.833    4.162   1.00  22.82      B
ATOM    2552   C    PRO B 146      41.597   19.945    5.933   1.00  22.63      B
ATOM    2553   O    PRO B 146      42.213   20.766    6.625   1.00  21.32      B
ATOM    2554   N    LEU B 147      40.667   19.146    6.445   1.00  22.60      B
ATOM    2555   CA   LEU B 147      40.414   19.142    7.883   1.00  22.34      B
ATOM    2556   CB   LEU B 147      39.241   18.216    8.213   1.00  22.17      B
ATOM    2557   CG   LEU B 147      38.934   17.973    9.691   1.00  24.53      B
ATOM    2558   CD1  LEU B 147      38.629   19.288   10.368   1.00  25.95      B
ATOM    2559   CD2  LEU B 147      37.746   17.026    9.826   1.00  25.55      B
ATOM    2560   C    LEU B 147      41.710   18.609    8.515   1.00  21.99      B
ATOM    2561   O    LEU B 147      42.290   17.640    8.024   1.00  21.35      B
ATOM    2562   N    ILE B 148      42.175   19.246    9.581   1.00  20.48      B
ATOM    2563   CA   ILE B 148      43.406   18.813   10.228   1.00  19.15      B
ATOM    2564   CB   ILE B 148      44.392   19.990   10.403   1.00  21.68      B
ATOM    2565   CG2  ILE B 148      45.666   19.505   11.065   1.00  20.10      B
ATOM    2566   CG1  ILE B 148      44.728   20.609    9.041   1.00  25.04      B
ATOM    2567   CD1  ILE B 148      45.416   19.649    8.090   1.00  29.06      B
ATOM    2568   C    ILE B 148      43.160   18.208   11.603   1.00  17.56      B
ATOM    2569   O    ILE B 148      42.566   18.852   12.467   1.00  14.88      B
ATOM    2570   N    ARG B 149      43.625   16.973   11.795   1.00  15.95      B
ATOM    2571   CA   ARG B 149      43.492   16.273   13.077   1.00  17.47      B
ATOM    2572   CB   ARG B 149      43.420   14.763   12.852   1.00  16.94      B
ATOM    2573   CG   ARG B 149      43.202   13.941   14.128   1.00  20.29      B
ATOM    2574   CD   ARG B 149      43.252   12.448   13.821   1.00  21.64      B
ATOM    2575   NE   ARG B 149      42.168   12.028   12.938   1.00  21.97      B
ATOM    2576   CZ   ARG B 149      40.934   11.742   13.348   1.00  23.22      B
ATOM    2577   NH1  ARG B 149      40.015   11.374   12.471   1.00  23.89      B
ATOM    2578   NH2  ARG B 149      40.623   11.803   14.636   1.00  23.11      B
ATOM    2579   C    ARG B 149      44.720   16.603   13.937   1.00  17.66      B
ATOM    2580   O    ARG B 149      45.850   16.311   13.549   1.00  17.51      B
ATOM    2581   N    ASN B 150      44.496   17.210   15.098   1.00  16.67      B
ATOM    2582   CA   ASN B 150      45.592   17.593   15.980   1.00  16.94      B
ATOM    2583   CB   ASN B 150      45.174   18.756   16.890   1.00  15.38      B
ATOM    2584   CG   ASN B 150      44.899   20.034   16.118   1.00  18.41      B
ATOM    2585   OD1  ASN B 150      45.685   20.436   15.249   1.00  19.05      B
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ATOM   2586  ND2 ASN B 150      43.790  20.691  16.440  1.00 17.88      B
ATOM   2587  C   ASN B 150      46.116  16.452  16.841  1.00 18.47      B
ATOM   2588  O   ASN B 150      47.220  16.540  17.384  1.00 17.03      B
ATOM   2589  N   GLY B 151      45.324  15.391  16.968  1.00 17.77      B
ATOM   2590  CA  GLY B 151      45.734  14.251  17.770  1.00 19.16      B
ATOM   2591  C   GLY B 151      45.258  14.293  19.213  1.00 20.44      B
ATOM   2592  O   GLY B 151      45.198  13.264  19.877  1.00 22.31      B
ATOM   2593  N   ASP B 152      44.906  15.475  19.701  1.00 20.79      B
ATOM   2594  CA  ASP B 152      44.450  15.624  21.077  1.00 21.97      B
ATOM   2595  CB  ASP B 152      45.192  16.790  21.748  1.00 21.95      B
ATOM   2596  CG  ASP B 152      45.027  18.101  20.992  1.00 28.05      B
ATOM   2597  OD1 ASP B 152      45.764  19.060  21.300  1.00 30.94      B
ATOM   2598  OD2 ASP B 152      44.158  18.181  20.090  1.00 28.02      B
ATOM   2599  C   ASP B 152      42.939  15.847  21.175  1.00 20.51      B
ATOM   2600  O   ASP B 152      42.474  16.619  22.010  1.00 21.63      B
ATOM   2601  N   TRP B 153      42.183  15.166  20.322  1.00 19.19      B
ATOM   2602  CA  TRP B 153      40.724  15.278  20.300  1.00 16.82      B
ATOM   2603  CB  TRP B 153      40.121  14.865  21.657  1.00 15.80      B
ATOM   2604  CG  TRP B 153      40.326  13.408  22.005  1.00 16.21      B
ATOM   2605  CD2 TRP B 153      39.415  12.322  21.756  1.00 16.58      B
ATOM   2606  CE2 TRP B 153      40.047  11.134  22.188  1.00 15.08      B
ATOM   2607  CE3 TRP B 153      38.125  12.238  21.211  1.00 15.69      B
ATOM   2608  CD1 TRP B 153      41.435  12.848  22.564  1.00 14.68      B
ATOM   2609  NE1 TRP B 153      41.278  11.483  22.677  1.00 15.53      B
ATOM   2610  CZ2 TRP B 153      39.438   9.879  22.087  1.00 15.60      B
ATOM   2611  CZ3 TRP B 153      37.518  10.987  21.112  1.00 14.22      B
ATOM   2612  CH2 TRP B 153      38.176   9.827  21.549  1.00 13.89      B
ATOM   2613  C   TRP B 153      40.194  16.660  19.890  1.00 16.09      B
ATOM   2614  O   TRP B 153      39.159  17.110  20.379  1.00 14.28      B
ATOM   2615  N   THR B 154      40.929  17.342  19.020  1.00 15.11      B
ATOM   2616  CA  THR B 154      40.499  18.627  18.483  1.00 16.19      B
ATOM   2617  CB  THR B 154      41.176  19.877  19.150  1.00 18.02      B
ATOM   2618  OG1 THR B 154      42.602  19.804  19.008  1.00 19.50      B
ATOM   2619  CG2 THR B 154      40.788  20.000  20.608  1.00 15.03      B
ATOM   2620  C   THR B 154      40.908  18.602  17.024  1.00 15.24      B
ATOM   2621  O   THR B 154      41.773  17.832  16.635  1.00 15.24      B
ATOM   2622  N   PHE B 155      40.269  19.437  16.220  1.00 18.04      B
ATOM   2623  CA  PHE B 155      40.577  19.538  14.801  1.00 16.03      B
ATOM   2624  CB  PHE B 155      39.404  19.042  13.938  1.00 16.98      B
ATOM   2625  CG  PHE B 155      39.069  17.579  14.118  1.00 17.58      B
ATOM   2626  CD1 PHE B 155      38.133  17.170  15.074  1.00 18.20      B
ATOM   2627  CD2 PHE B 155      39.670  16.611  13.312  1.00 17.71      B
ATOM   2628  CE1 PHE B 155      37.799  15.810  15.223  1.00 17.81      B
ATOM   2629  CE2 PHE B 155      39.346  15.250  13.451  1.00 17.57      B
ATOM   2630  CZ  PHE B 155      38.407  14.849  14.409  1.00 16.39      B
ATOM   2631  C   PHE B 155      40.793  21.015  14.503  1.00 16.67      B
ATOM   2632  O   PHE B 155      40.532  21.870  15.352  1.00 16.84      B
ATOM   2633  N   GLN B 156      41.281  21.312  13.304  1.00 14.72      B
ATOM   2634  CA  GLN B 156      41.467  22.689  12.886  1.00 14.66      B
ATOM   2635  CB  GLN B 156      42.811  23.264  13.357  1.00 16.69      B
ATOM   2636  CG  GLN B 156      44.039  22.698  12.669  1.00 15.65      B
ATOM   2637  CD  GLN B 156      45.292  23.486  13.011  1.00 17.87      B
ATOM   2638  OE1 GLN B 156      45.477  24.617  12.555  1.00 17.56      B
ATOM   2639  NE2 GLN B 156      46.153  22.897  13.830  1.00 15.40      B
ATOM   2640  C   GLN B 156      41.398  22.722  11.371  1.00 14.00      B
ATOM   2641  O   GLN B 156      41.477  21.691  10.716  1.00 15.17      B
ATOM   2642  N   ILE B 157      41.241  23.911  10.818  1.00 15.34      B
ATOM   2643  CA  ILE B 157      41.165  24.057   9.383  1.00 17.26      B
ATOM   2644  CB  ILE B 157      39.791  23.585   8.856  1.00 16.56      B
ATOM   2645  CG2 ILE B 157      38.675  24.429   9.474  1.00 13.07      B
ATOM   2646  CG1 ILE B 157      39.765  23.649   7.326  1.00 17.72      B
ATOM   2647  CD1 ILE B 157      38.583  22.913   6.712  1.00 14.50      B
ATOM   2648  C   ILE B 157      41.379  25.523   9.074  1.00 18.67      B
ATOM   2649  O   ILE B 157      40.823  26.391   9.745  1.00 22.28      B
ATOM   2650  N   LEU B 158      42.217  25.795   8.083  1.00 18.98      B
ATOM   2651  CA  LEU B 158      42.508  27.162   7.690  1.00 20.77      B
ATOM   2652  CB  LEU B 158      44.022  27.368   7.555  1.00 22.23      B
ATOM   2653  CG  LEU B 158      44.851  27.525   8.838  1.00 26.12      B
ATOM   2654  CD1 LEU B 158      44.689  26.320   9.740  1.00 29.01      B
ATOM   2655  CD2 LEU B 158      46.311  27.701   8.465  1.00 28.46      B
ATOM   2656  C   LEU B 158      41.817  27.484   6.371  1.00 20.61      B
ATOM   2657  O   LEU B 158      41.934  26.734   5.401  1.00 19.39      B
ATOM   2658  N   VAL B 159      41.088  28.596   6.346  1.00 21.67      B
ATOM   2659  CA  VAL B 159      40.380  29.011   5.141  1.00 21.90      B
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| ATOM | 2660 | CB | VAL B 159 | 38.855 | 29.061 | 5.365 | 1.00 22.06 | B |
|---|---|---|---|---|---|---|---|---|
| ATOM | 2661 | CG1 | VAL B 159 | 38.147 | 29.252 | 4.043 | 1.00 20.55 | B |
| ATOM | 2662 | CG2 | VAL B 159 | 38.381 | 27.766 | 6.009 | 1.00 20.83 | B |
| ATOM | 2663 | C | VAL B 159 | 40.899 | 30.379 | 4.749 | 1.00 21.80 | B |
| ATOM | 2664 | O | VAL B 159 | 40.721 | 31.357 | 5.473 | 1.00 20.82 | B |
| ATOM | 2665 | N | MET B 160 | 41.555 | 30.416 | 3.592 | 1.00 23.56 | B |
| ATOM | 2666 | CA | MET B 160 | 42.179 | 31.613 | 3.055 | 1.00 25.12 | B |
| ATOM | 2667 | CB | MET B 160 | 43.580 | 31.257 | 2.559 | 1.00 26.80 | B |
| ATOM | 2668 | CG | MET B 160 | 44.479 | 30.736 | 3.678 | 1.00 32.00 | B |
| ATOM | 2669 | SD | MET B 160 | 45.850 | 29.700 | 3.145 | 1.00 38.02 | B |
| ATOM | 2670 | CE | MET B 160 | 45.094 | 28.065 | 3.307 | 1.00 35.43 | B |
| ATOM | 2671 | C | MET B 160 | 41.387 | 32.269 | 1.941 | 1.00 28.27 | B |
| ATOM | 2672 | O | MET B 160 | 40.684 | 31.602 | 1.177 | 1.00 28.76 | B |
| ATOM | 2673 | N | LEU B 161 | 41.518 | 33.588 | 1.854 | 1.00 29.59 | B |
| ATOM | 2674 | CA | LEU B 161 | 40.820 | 34.366 | 0.845 | 1.00 32.69 | B |
| ATOM | 2675 | CB | LEU B 161 | 39.669 | 35.142 | 1.487 | 1.00 30.80 | B |
| ATOM | 2676 | CG | LEU B 161 | 39.031 | 36.199 | 0.586 | 1.00 31.56 | B |
| ATOM | 2677 | CD1 | LEU B 161 | 38.156 | 35.516 | -0.460 | 1.00 29.64 | B |
| ATOM | 2678 | CD2 | LEU B 161 | 38.213 | 37.167 | 1.423 | 1.00 29.89 | B |
| ATOM | 2679 | C | LEU B 161 | 41.755 | 35.349 | 0.154 | 1.00 35.59 | B |
| ATOM | 2680 | O | LEU B 161 | 42.350 | 36.216 | 0.801 | 1.00 35.54 | B |
| ATOM | 2681 | N | GLU B 162 | 41.895 | 35.203 | -1.158 | 1.00 39.87 | B |
| ATOM | 2682 | CA | GLU B 162 | 42.728 | 36.118 | -1.927 | 1.00 44.05 | B |
| ATOM | 2683 | CB | GLU B 162 | 42.995 | 35.565 | -3.331 | 1.00 46.86 | B |
| ATOM | 2684 | CG | GLU B 162 | 43.795 | 36.497 | -4.239 | 1.00 50.98 | B |
| ATOM | 2685 | CD | GLU B 162 | 45.274 | 36.537 | -3.891 | 1.00 54.75 | B |
| ATOM | 2686 | OE1 | GLU B 162 | 45.604 | 36.802 | -2.715 | 1.00 56.53 | B |
| ATOM | 2687 | OE2 | GLU B 162 | 46.108 | 36.308 | -4.796 | 1.00 55.16 | B |
| ATOM | 2688 | C | GLU B 162 | 41.879 | 37.372 | -2.029 | 1.00 44.69 | B |
| ATOM | 2689 | O | GLU B 162 | 40.719 | 37.302 | -2.434 | 1.00 44.39 | B |
| ATOM | 2690 | N | MET B 163 | 42.436 | 38.514 | -1.648 | 1.00 46.67 | B |
| ATOM | 2691 | CA | MET B 163 | 41.670 | 39.746 | -1.716 | 1.00 49.56 | B |
| ATOM | 2692 | CB | MET B 163 | 40.881 | 39.949 | -0.412 | 1.00 51.22 | B |
| ATOM | 2693 | CG | MET B 163 | 41.652 | 39.675 | 0.876 | 1.00 51.58 | B |
| ATOM | 2694 | SD | MET B 163 | 42.910 | 40.901 | 1.274 | 1.00 56.87 | B |
| ATOM | 2695 | CE | MET B 163 | 41.915 | 42.187 | 2.029 | 1.00 54.89 | B |
| ATOM | 2696 | C | MET B 163 | 42.487 | 40.986 | -2.028 | 1.00 51.43 | B |
| ATOM | 2697 | O | MET B 163 | 43.717 | 40.988 | -1.942 | 1.00 51.02 | B |
| ATOM | 2698 | N | THR B 164 | 41.777 | 42.038 | -2.412 | 1.00 53.70 | B |
| ATOM | 2699 | CA | THR B 164 | 42.385 | 43.316 | -2.738 | 1.00 56.61 | B |
| ATOM | 2700 | CB | THR B 164 | 41.889 | 43.820 | -4.116 | 1.00 57.48 | B |
| ATOM | 2701 | OG1 | THR B 164 | 40.457 | 43.744 | -4.172 | 1.00 57.81 | B |
| ATOM | 2702 | CG2 | THR B 164 | 42.480 | 42.967 | -5.234 | 1.00 57.23 | B |
| ATOM | 2703 | C | THR B 164 | 42.012 | 44.318 | -1.642 | 1.00 57.80 | B |
| ATOM | 2704 | O | THR B 164 | 40.866 | 44.766 | -1.555 | 1.00 57.08 | B |
| ATOM | 2705 | N | PRO B 165 | 42.976 | 44.658 | -0.770 | 1.00 58.98 | B |
| ATOM | 2706 | CD | PRO B 165 | 44.315 | 44.055 | -0.647 | 1.00 59.54 | B |
| ATOM | 2707 | CA | PRO B 165 | 42.734 | 45.605 | 0.322 | 1.00 60.52 | B |
| ATOM | 2708 | CB | PRO B 165 | 44.063 | 45.608 | 1.078 | 1.00 60.33 | B |
| ATOM | 2709 | CG | PRO B 165 | 44.604 | 44.236 | 0.822 | 1.00 60.42 | B |
| ATOM | 2710 | C | PRO B 165 | 42.347 | 47.002 | -0.163 | 1.00 61.65 | B |
| ATOM | 2711 | O | PRO B 165 | 43.149 | 47.698 | -0.790 | 1.00 61.24 | B |
| ATOM | 2712 | N | GLN B 166 | 41.110 | 47.395 | 0.126 | 1.00 62.45 | B |
| ATOM | 2713 | CA | GLN B 166 | 40.598 | 48.709 | -0.250 | 1.00 63.32 | B |
| ATOM | 2714 | CB | GLN B 166 | 39.605 | 48.590 | -1.410 | 1.00 65.46 | B |
| ATOM | 2715 | CG | GLN B 166 | 40.177 | 47.945 | -2.661 | 1.00 69.00 | B |
| ATOM | 2716 | CD | GLN B 166 | 39.195 | 47.942 | -3.819 | 1.00 71.19 | B |
| ATOM | 2717 | OE1 | GLN B 166 | 38.071 | 47.448 | -3.697 | 1.00 72.48 | B |
| ATOM | 2718 | NE2 | GLN B 166 | 39.617 | 48.492 | -4.954 | 1.00 72.65 | B |
| ATOM | 2719 | C | GLN B 166 | 39.893 | 49.287 | 0.970 | 1.00 62.65 | B |
| ATOM | 2720 | O | GLN B 166 | 39.021 | 48.635 | 1.550 | 1.00 62.16 | B |
| ATOM | 2721 | N | ARG B 167 | 40.266 | 50.501 | 1.366 | 1.00 61.62 | B |
| ATOM | 2722 | CA | ARG B 167 | 39.645 | 51.111 | 2.535 | 1.00 60.86 | B |
| ATOM | 2723 | CB | ARG B 167 | 40.190 | 52.525 | 2.777 | 1.00 62.57 | B |
| ATOM | 2724 | CG | ARG B 167 | 39.953 | 53.029 | 4.204 | 1.00 64.82 | B |
| ATOM | 2725 | CD | ARG B 167 | 40.742 | 52.198 | 5.227 | 1.00 67.31 | B |
| ATOM | 2726 | NE | ARG B 167 | 40.094 | 52.143 | 6.539 | 1.00 69.03 | B |
| ATOM | 2727 | CZ | ARG B 167 | 40.570 | 51.477 | 7.591 | 1.00 69.14 | B |
| ATOM | 2728 | NH1 | ARG B 167 | 41.710 | 50.804 | 7.499 | 1.00 69.34 | B |
| ATOM | 2729 | NH2 | ARG B 167 | 39.897 | 51.471 | 8.735 | 1.00 69.52 | B |
| ATOM | 2730 | C | ARG B 167 | 38.136 | 51.154 | 2.333 | 1.00 59.19 | B |
| ATOM | 2731 | O | ARG B 167 | 37.647 | 51.615 | 1.303 | 1.00 58.60 | B |
| ATOM | 2732 | N | GLY B 168 | 37.404 | 50.656 | 3.320 | 1.00 58.18 | B |
| ATOM | 2733 | CA | GLY B 168 | 35.959 | 50.632 | 3.226 | 1.00 56.57 | B |

| ATOM | 2734 | C | GLY | B | 168 | 35.466 | 49.200 | 3.191 | 1.00 | 55.42 | B |
|------|------|------|------|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2735 | O | GLY | B | 168 | 34.306 | 48.924 | 3.495 | 1.00 | 55.98 | B |
| ATOM | 2736 | N | ASP | B | 169 | 36.350 | 48.280 | 2.814 | 1.00 | 53.44 | B |
| ATOM | 2737 | CA | ASP | B | 169 | 35.979 | 46.871 | 2.757 | 1.00 | 51.76 | B |
| ATOM | 2738 | CB | ASP | B | 169 | 36.841 | 46.115 | 1.740 | 1.00 | 50.49 | B |
| ATOM | 2739 | CG | ASP | B | 169 | 36.428 | 46.392 | 0.311 | 1.00 | 50.57 | B |
| ATOM | 2740 | OD1 | ASP | B | 169 | 35.207 | 46.479 | 0.060 | 1.00 | 49.92 | B |
| ATOM | 2741 | OD2 | ASP | B | 169 | 37.318 | 46.507 | -0.559 | 1.00 | 49.84 | B |
| ATOM | 2742 | C | ASP | B | 169 | 36.083 | 46.181 | 4.110 | 1.00 | 49.36 | B |
| ATOM | 2743 | O | ASP | B | 169 | 37.066 | 46.343 | 4.836 | 1.00 | 48.92 | B |
| ATOM | 2744 | N | VAL | B | 170 | 35.047 | 45.418 | 4.436 | 1.00 | 47.48 | B |
| ATOM | 2745 | CA | VAL | B | 170 | 34.981 | 44.667 | 5.680 | 1.00 | 45.10 | B |
| ATOM | 2746 | CB | VAL | B | 170 | 33.800 | 45.130 | 6.543 | 1.00 | 45.86 | B |
| ATOM | 2747 | CG1 | VAL | B | 170 | 33.702 | 44.268 | 7.795 | 1.00 | 46.26 | B |
| ATOM | 2748 | CG2 | VAL | B | 170 | 33.974 | 46.598 | 6.906 | 1.00 | 46.23 | B |
| ATOM | 2749 | C | VAL | B | 170 | 34.787 | 43.191 | 5.342 | 1.00 | 43.62 | B |
| ATOM | 2750 | O | VAL | B | 170 | 33.774 | 42.807 | 4.762 | 1.00 | 42.86 | B |
| ATOM | 2751 | N | TYR | B | 171 | 35.762 | 42.367 | 5.704 | 1.00 | 41.69 | B |
| ATOM | 2752 | CA | TYR | B | 171 | 35.694 | 40.935 | 5.425 | 1.00 | 38.95 | B |
| ATOM | 2753 | CB | TYR | B | 171 | 37.044 | 40.455 | 4.899 | 1.00 | 37.52 | B |
| ATOM | 2754 | CG | TYR | B | 171 | 37.405 | 41.031 | 3.553 | 1.00 | 38.12 | B |
| ATOM | 2755 | CD1 | TYR | B | 171 | 37.023 | 40.391 | 2.376 | 1.00 | 37.52 | B |
| ATOM | 2756 | CE1 | TYR | B | 171 | 37.342 | 40.923 | 1.131 | 1.00 | 38.06 | B |
| ATOM | 2757 | CD2 | TYR | B | 171 | 38.118 | 42.224 | 3.454 | 1.00 | 37.54 | B |
| ATOM | 2758 | CE2 | TYR | B | 171 | 38.442 | 42.767 | 2.216 | 1.00 | 38.45 | B |
| ATOM | 2759 | CZ | TYR | B | 171 | 38.052 | 42.110 | 1.056 | 1.00 | 39.25 | B |
| ATOM | 2760 | OH | TYR | B | 171 | 38.372 | 42.641 | -0.172 | 1.00 | 38.84 | B |
| ATOM | 2761 | C | TYR | B | 171 | 35.314 | 40.139 | 6.671 | 1.00 | 37.46 | B |
| ATOM | 2762 | O | TYR | B | 171 | 35.791 | 40.428 | 7.773 | 1.00 | 34.85 | B |
| ATOM | 2763 | N | THR | B | 172 | 34.452 | 39.140 | 6.501 | 1.00 | 35.06 | B |
| ATOM | 2764 | CA | THR | B | 172 | 34.049 | 38.328 | 7.638 | 1.00 | 35.81 | B |
| ATOM | 2765 | CB | THR | B | 172 | 32.589 | 38.622 | 8.064 | 1.00 | 38.37 | B |
| ATOM | 2766 | OG1 | THR | B | 172 | 31.688 | 38.177 | 7.043 | 1.00 | 42.02 | B |
| ATOM | 2767 | CG2 | THR | B | 172 | 32.390 | 40.119 | 8.292 | 1.00 | 39.83 | B |
| ATOM | 2768 | C | THR | B | 172 | 34.182 | 36.830 | 7.406 | 1.00 | 33.71 | B |
| ATOM | 2769 | O | THR | B | 172 | 33.953 | 36.335 | 6.300 | 1.00 | 32.99 | B |
| ATOM | 2770 | N | CYS | B | 173 | 34.578 | 36.123 | 8.463 | 1.00 | 32.09 | B |
| ATOM | 2771 | CA | CYS | B | 173 | 34.714 | 34.670 | 8.438 | 1.00 | 31.08 | B |
| ATOM | 2772 | C | CYS | B | 173 | 33.497 | 34.183 | 9.200 | 1.00 | 30.92 | B |
| ATOM | 2773 | O | CYS | B | 173 | 33.240 | 34.614 | 10.326 | 1.00 | 32.70 | B |
| ATOM | 2774 | CB | CYS | B | 173 | 35.988 | 34.214 | 9.155 | 1.00 | 31.48 | B |
| ATOM | 2775 | SG | CYS | B | 173 | 36.338 | 32.436 | 8.983 | 1.00 | 31.85 | B |
| ATOM | 2776 | N | HIS | B | 174 | 32.748 | 33.288 | 8.578 | 1.00 | 30.26 | B |
| ATOM | 2777 | CA | HIS | B | 174 | 31.524 | 32.754 | 9.152 | 1.00 | 29.72 | B |
| ATOM | 2778 | CB | HIS | B | 174 | 30.401 | 32.977 | 8.128 | 1.00 | 30.80 | B |
| ATOM | 2779 | CG | HIS | B | 174 | 29.030 | 32.625 | 8.615 | 1.00 | 32.90 | B |
| ATOM | 2780 | CD2 | HIS | B | 174 | 28.016 | 33.405 | 9.058 | 1.00 | 33.11 | B |
| ATOM | 2781 | ND1 | HIS | B | 174 | 28.551 | 31.332 | 8.621 | 1.00 | 34.85 | B |
| ATOM | 2782 | CE1 | HIS | B | 174 | 27.299 | 31.332 | 9.044 | 1.00 | 37.21 | B |
| ATOM | 2783 | NE2 | HIS | B | 174 | 26.950 | 32.577 | 9.316 | 1.00 | 34.95 | B |
| ATOM | 2784 | C | HIS | B | 174 | 31.751 | 31.271 | 9.449 | 1.00 | 28.49 | B |
| ATOM | 2785 | O | HIS | B | 174 | 32.080 | 30.494 | 8.554 | 1.00 | 27.69 | B |
| ATOM | 2786 | N | VAL | B | 175 | 31.584 | 30.888 | 10.710 | 1.00 | 27.48 | B |
| ATOM | 2787 | CA | VAL | B | 175 | 31.810 | 29.508 | 11.121 | 1.00 | 25.94 | B |
| ATOM | 2788 | CB | VAL | B | 175 | 32.988 | 29.418 | 12.126 | 1.00 | 25.31 | B |
| ATOM | 2789 | CG1 | VAL | B | 175 | 33.147 | 27.982 | 12.629 | 1.00 | 21.10 | B |
| ATOM | 2790 | CG2 | VAL | B | 175 | 34.271 | 29.896 | 11.462 | 1.00 | 22.12 | B |
| ATOM | 2791 | C | VAL | B | 175 | 30.606 | 28.821 | 11.748 | 1.00 | 26.58 | B |
| ATOM | 2792 | O | VAL | B | 175 | 30.004 | 29.328 | 12.694 | 1.00 | 27.01 | B |
| ATOM | 2793 | N | GLU | B | 176 | 30.274 | 27.652 | 11.212 | 1.00 | 27.17 | B |
| ATOM | 2794 | CA | GLU | B | 176 | 29.168 | 26.846 | 11.712 | 1.00 | 28.51 | B |
| ATOM | 2795 | CB | GLU | B | 176 | 28.166 | 26.573 | 10.588 | 1.00 | 32.35 | B |
| ATOM | 2796 | CG | GLU | B | 176 | 27.454 | 27.827 | 10.082 | 1.00 | 38.87 | B |
| ATOM | 2797 | CD | GLU | B | 176 | 26.776 | 27.616 | 8.735 | 1.00 | 42.45 | B |
| ATOM | 2798 | OE1 | GLU | B | 176 | 25.947 | 26.684 | 8.618 | 1.00 | 43.07 | B |
| ATOM | 2799 | OE2 | GLU | B | 176 | 27.075 | 28.386 | 7.794 | 1.00 | 42.94 | B |
| ATOM | 2800 | C | GLU | B | 176 | 29.750 | 25.536 | 12.235 | 1.00 | 27.34 | B |
| ATOM | 2801 | O | GLU | B | 176 | 30.576 | 24.900 | 11.574 | 1.00 | 26.12 | B |
| ATOM | 2802 | N | HIS | B | 177 | 29.308 | 25.134 | 13.420 | 1.00 | 26.08 | B |
| ATOM | 2803 | CA | HIS | B | 177 | 29.800 | 23.921 | 14.049 | 1.00 | 26.30 | B |
| ATOM | 2804 | CB | HIS | B | 177 | 31.132 | 24.244 | 14.738 | 1.00 | 24.58 | B |
| ATOM | 2805 | CG | HIS | B | 177 | 31.759 | 23.076 | 15.422 | 1.00 | 22.32 | B |
| ATOM | 2806 | CD2 | HIS | B | 177 | 32.646 | 22.156 | 14.977 | 1.00 | 21.05 | B |
| ATOM | 2807 | ND1 | HIS | B | 177 | 31.437 | 22.711 | 16.710 | 1.00 | 21.01 | B |

| ATOM | 2808 | CE1 | HIS | B | 177 | 32.097 | 21.613 | 17.030 | 1.00 | 23.72 | B |
| ATOM | 2809 | NE2 | HIS | B | 177 | 32.838 | 21.255 | 15.995 | 1.00 | 23.87 | B |
| ATOM | 2810 | C | HIS | B | 177 | 28.762 | 23.413 | 15.057 | 1.00 | 27.87 | B |
| ATOM | 2811 | O | HIS | B | 177 | 28.059 | 24.205 | 15.672 | 1.00 | 29.54 | B |
| ATOM | 2812 | N | PRO | B | 178 | 28.654 | 22.085 | 15.237 | 1.00 | 29.57 | B |
| ATOM | 2813 | CD | PRO | B | 178 | 29.365 | 21.025 | 14.501 | 1.00 | 28.96 | B |
| ATOM | 2814 | CA | PRO | B | 178 | 27.687 | 21.497 | 16.175 | 1.00 | 31.71 | B |
| ATOM | 2815 | CB | PRO | B | 178 | 28.062 | 20.019 | 16.166 | 1.00 | 30.49 | B |
| ATOM | 2816 | CG | PRO | B | 178 | 28.503 | 19.810 | 14.769 | 1.00 | 30.01 | B |
| ATOM | 2817 | C | PRO | B | 178 | 27.649 | 22.071 | 17.595 | 1.00 | 33.29 | B |
| ATOM | 2818 | O | PRO | B | 178 | 26.619 | 22.020 | 18.256 | 1.00 | 35.00 | B |
| ATOM | 2819 | N | SER | B | 179 | 28.762 | 22.615 | 18.067 | 1.00 | 34.96 | B |
| ATOM | 2820 | CA | SER | B | 179 | 28.813 | 23.168 | 19.418 | 1.00 | 36.85 | B |
| ATOM | 2821 | CB | SER | B | 179 | 30.261 | 23.228 | 19.896 | 1.00 | 35.35 | B |
| ATOM | 2822 | OG | SER | B | 179 | 31.023 | 24.053 | 19.034 | 1.00 | 35.14 | B |
| ATOM | 2823 | C | SER | B | 179 | 28.206 | 24.564 | 19.522 | 1.00 | 38.40 | B |
| ATOM | 2824 | O | SER | B | 179 | 27.953 | 25.056 | 20.619 | 1.00 | 37.27 | B |
| ATOM | 2825 | N | LEU | B | 180 | 27.971 | 25.192 | 18.377 | 1.00 | 40.10 | B |
| ATOM | 2826 | CA | LEU | B | 180 | 27.434 | 26.545 | 18.340 | 1.00 | 41.36 | B |
| ATOM | 2827 | CB | LEU | B | 180 | 28.162 | 27.352 | 17.269 | 1.00 | 39.74 | B |
| ATOM | 2828 | CG | LEU | B | 180 | 29.677 | 27.432 | 17.422 | 1.00 | 39.93 | B |
| ATOM | 2829 | CD1 | LEU | B | 180 | 30.286 | 28.013 | 16.157 | 1.00 | 39.41 | B |
| ATOM | 2830 | CD2 | LEU | B | 180 | 30.021 | 28.279 | 18.636 | 1.00 | 39.61 | B |
| ATOM | 2831 | C | LEU | B | 180 | 25.944 | 26.633 | 18.078 | 1.00 | 43.85 | B |
| ATOM | 2832 | O | LEU | B | 180 | 25.449 | 26.125 | 17.072 | 1.00 | 44.25 | B |
| ATOM | 2833 | N | GLN | B | 181 | 25.230 | 27.289 | 18.984 | 1.00 | 47.20 | B |
| ATOM | 2834 | CA | GLN | B | 181 | 23.794 | 27.475 | 18.814 | 1.00 | 49.93 | B |
| ATOM | 2835 | CB | GLN | B | 181 | 23.158 | 27.956 | 20.121 | 1.00 | 52.00 | B |
| ATOM | 2836 | CG | GLN | B | 181 | 23.873 | 29.134 | 20.758 | 1.00 | 56.40 | B |
| ATOM | 2837 | CD | GLN | B | 181 | 23.263 | 29.538 | 22.084 | 1.00 | 59.03 | B |
| ATOM | 2838 | OE1 | GLN | B | 181 | 22.087 | 29.908 | 22.153 | 1.00 | 60.55 | B |
| ATOM | 2839 | NE2 | GLN | B | 181 | 24.059 | 29.468 | 23.149 | 1.00 | 58.44 | B |
| ATOM | 2840 | C | GLN | B | 181 | 23.635 | 28.522 | 17.715 | 1.00 | 49.23 | B |
| ATOM | 2841 | O | GLN | B | 181 | 22.712 | 28.465 | 16.906 | 1.00 | 49.91 | B |
| ATOM | 2842 | N | SER | B | 182 | 24.560 | 29.474 | 17.688 | 1.00 | 48.48 | B |
| ATOM | 2843 | CA | SER | B | 182 | 24.555 | 30.523 | 16.679 | 1.00 | 47.89 | B |
| ATOM | 2844 | CB | SER | B | 182 | 24.241 | 31.879 | 17.314 | 1.00 | 48.68 | B |
| ATOM | 2845 | OG | SER | B | 182 | 25.211 | 32.223 | 18.286 | 1.00 | 50.58 | B |
| ATOM | 2846 | C | SER | B | 182 | 25.938 | 30.550 | 16.038 | 1.00 | 45.93 | B |
| ATOM | 2847 | O | SER | B | 182 | 26.945 | 30.354 | 16.714 | 1.00 | 45.13 | B |
| ATOM | 2848 | N | PRO | B | 183 | 26.004 | 30.783 | 14.721 | 1.00 | 45.12 | B |
| ATOM | 2849 | CD | PRO | B | 183 | 24.911 | 31.096 | 13.784 | 1.00 | 44.93 | B |
| ATOM | 2850 | CA | PRO | B | 183 | 27.302 | 30.819 | 14.042 | 1.00 | 43.29 | B |
| ATOM | 2851 | CB | PRO | B | 183 | 26.923 | 31.070 | 12.581 | 1.00 | 43.70 | B |
| ATOM | 2852 | CG | PRO | B | 183 | 25.642 | 31.833 | 12.688 | 1.00 | 44.70 | B |
| ATOM | 2853 | C | PRO | B | 183 | 28.254 | 31.876 | 14.593 | 1.00 | 40.67 | B |
| ATOM | 2854 | O | PRO | B | 183 | 27.828 | 32.851 | 15.209 | 1.00 | 40.46 | B |
| ATOM | 2855 | N | ILE | B | 184 | 29.547 | 31.664 | 14.382 | 1.00 | 37.76 | B |
| ATOM | 2856 | CA | ILE | B | 184 | 30.550 | 32.607 | 14.842 | 1.00 | 35.88 | B |
| ATOM | 2857 | CB | ILE | B | 184 | 31.759 | 31.889 | 15.468 | 1.00 | 35.92 | B |
| ATOM | 2858 | CG2 | ILE | B | 184 | 32.907 | 32.867 | 15.657 | 1.00 | 35.57 | B |
| ATOM | 2859 | CG1 | ILE | B | 184 | 31.362 | 31.270 | 16.806 | 1.00 | 36.74 | B |
| ATOM | 2860 | CD1 | ILE | B | 184 | 32.475 | 30.477 | 17.458 | 1.00 | 36.59 | B |
| ATOM | 2861 | C | ILE | B | 184 | 31.040 | 33.453 | 13.680 | 1.00 | 34.88 | B |
| ATOM | 2862 | O | ILE | B | 184 | 31.412 | 32.932 | 12.630 | 1.00 | 35.06 | B |
| ATOM | 2863 | N | THR | B | 185 | 31.043 | 34.764 | 13.876 | 1.00 | 34.50 | B |
| ATOM | 2864 | CA | THR | B | 185 | 31.500 | 35.675 | 12.845 | 1.00 | 34.32 | B |
| ATOM | 2865 | CB | THR | B | 185 | 30.356 | 36.592 | 12.341 | 1.00 | 35.40 | B |
| ATOM | 2866 | OG1 | THR | B | 185 | 29.770 | 37.285 | 13.450 | 1.00 | 37.01 | B |
| ATOM | 2867 | CG2 | THR | B | 185 | 29.286 | 35.774 | 11.631 | 1.00 | 35.73 | B |
| ATOM | 2868 | C | THR | B | 185 | 32.622 | 36.548 | 13.375 | 1.00 | 33.38 | B |
| ATOM | 2869 | O | THR | B | 185 | 32.559 | 37.050 | 14.494 | 1.00 | 32.86 | B |
| ATOM | 2870 | N | VAL | B | 186 | 33.652 | 36.713 | 12.560 | 1.00 | 32.69 | B |
| ATOM | 2871 | CA | VAL | B | 186 | 34.791 | 37.538 | 12.911 | 1.00 | 33.21 | B |
| ATOM | 2872 | CB | VAL | B | 186 | 36.041 | 36.683 | 13.155 | 1.00 | 33.39 | B |
| ATOM | 2873 | CG1 | VAL | B | 186 | 37.212 | 37.570 | 13.516 | 1.00 | 33.93 | B |
| ATOM | 2874 | CG2 | VAL | B | 186 | 35.766 | 35.674 | 14.262 | 1.00 | 33.67 | B |
| ATOM | 2875 | C | VAL | B | 186 | 35.023 | 38.454 | 11.721 | 1.00 | 34.68 | B |
| ATOM | 2876 | O | VAL | B | 186 | 35.060 | 37.997 | 10.579 | 1.00 | 32.50 | B |
| ATOM | 2877 | N | GLU | B | 187 | 35.172 | 39.746 | 11.988 | 1.00 | 36.30 | B |
| ATOM | 2878 | CA | GLU | B | 187 | 35.373 | 40.713 | 10.922 | 1.00 | 38.96 | B |
| ATOM | 2879 | CB | GLU | B | 187 | 34.484 | 41.937 | 11.154 | 1.00 | 40.90 | B |
| ATOM | 2880 | CG | GLU | B | 187 | 33.008 | 41.623 | 11.333 | 1.00 | 46.09 | B |
| ATOM | 2881 | CD | GLU | B | 187 | 32.146 | 42.876 | 11.421 | 1.00 | 48.81 | B |

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ATOM   2882  OE1 GLU B 187      30.909  42.739  11.545  1.00 51.77      B
ATOM   2883  OE2 GLU B 187      32.701  43.997  11.363  1.00 49.79      B
ATOM   2884  C   GLU B 187      36.816  41.175  10.784  1.00 39.59      B
ATOM   2885  O   GLU B 187      37.637  40.998  11.684  1.00 39.84      B
ATOM   2886  N   TRP B 188      37.113  41.765   9.635  1.00 39.59      B
ATOM   2887  CA  TRP B 188      38.430  42.302   9.360  1.00 40.86      B
ATOM   2888  CB  TRP B 188      39.339  41.252   8.736  1.00 38.70      B
ATOM   2889  CG  TRP B 188      40.769  41.704   8.693  1.00 37.82      B
ATOM   2890  CD2 TRP B 188      41.421  42.383   7.615  1.00 36.62      B
ATOM   2891  CE2 TRP B 188      42.748  42.640   8.023  1.00 36.31      B
ATOM   2892  CE3 TRP B 188      41.013  42.799   6.340  1.00 36.14      B
ATOM   2893  CD1 TRP B 188      41.698  41.583   9.686  1.00 37.31      B
ATOM   2894  NE1 TRP B 188      42.890  42.141   9.291  1.00 37.27      B
ATOM   2895  CZ2 TRP B 188      43.673  43.296   7.204  1.00 37.17      B
ATOM   2896  CZ3 TRP B 188      41.932  43.452   5.522  1.00 38.70      B
ATOM   2897  CH2 TRP B 188      43.249  43.694   5.960  1.00 37.13      B
ATOM   2898  C   TRP B 188      38.258  43.455   8.383  1.00 42.97      B
ATOM   2899  O   TRP B 188      37.946  43.240   7.211  1.00 42.37      B
ATOM   2900  N   ARG B 189      38.442  44.678   8.864  1.00 46.69      B
ATOM   2901  CA  ARG B 189      38.303  45.842   7.999  1.00 50.32      B
ATOM   2902  CB  ARG B 189      37.731  47.040   8.776  1.00 52.18      B
ATOM   2903  CG  ARG B 189      38.615  47.590   9.893  1.00 56.00      B
ATOM   2904  CD  ARG B 189      38.234  47.041  11.270  1.00 59.95      B
ATOM   2905  NE  ARG B 189      38.639  45.650  11.479  1.00 63.62      B
ATOM   2906  CZ  ARG B 189      39.903  45.236  11.559  1.00 64.33      B
ATOM   2907  NH1 ARG B 189      40.899  46.105  11.447  1.00 65.45      B
ATOM   2908  NH2 ARG B 189      40.172  43.951  11.760  1.00 64.46      B
ATOM   2909  C   ARG B 189      39.664  46.192   7.412  1.00 50.56      B
ATOM   2910  O   ARG B 189      40.680  46.119   8.100  1.00 50.34      B
ATOM   2911  N   ALA B 190      39.684  46.554   6.135  1.00 52.30      B
ATOM   2912  CA  ALA B 190      40.933  46.911   5.476  1.00 54.16      B
ATOM   2913  CB  ALA B 190      40.846  46.592   3.987  1.00 55.33      B
ATOM   2914  C   ALA B 190      41.238  48.392   5.679  1.00 55.19      B
ATOM   2915  O   ALA B 190      40.300  49.147   6.023  1.00 54.90      B
ATOM   2916  OXT ALA B 190      42.408  48.782   5.481  1.00 56.19      B
ATOM   2917  C   LEU C   1      32.073   1.033  33.225  1.00 35.70      C
ATOM   2918  O   LEU C   1      33.091   1.607  33.619  1.00 35.87      C
ATOM   2919  N   LEU C   1      29.791   1.906  32.702  1.00 36.17      C
ATOM   2920  CA  LEU C   1      30.699   1.409  33.777  1.00 34.35      C
ATOM   2921  N   GLN C   2      32.105   0.072  32.307  1.00 34.64      C
ATOM   2922  CA  GLN C   2      33.374  -0.359  31.737  1.00 34.20      C
ATOM   2923  C   GLN C   2      33.250  -0.823  30.294  1.00 33.55      C
ATOM   2924  O   GLN C   2      32.373  -1.610  29.955  1.00 33.68      C
ATOM   2925  N   PRO C   3      34.130  -0.329  29.418  1.00 33.74      C
ATOM   2926  CD  PRO C   3      35.226   0.632  29.639  1.00 33.81      C
ATOM   2927  CA  PRO C   3      34.064  -0.742  28.015  1.00 34.77      C
ATOM   2928  CB  PRO C   3      35.027   0.222  27.329  1.00 34.33      C
ATOM   2929  CG  PRO C   3      36.070   0.449  28.393  1.00 34.78      C
ATOM   2930  C   PRO C   3      34.508  -2.195  27.890  1.00 34.42      C
ATOM   2931  O   PRO C   3      35.435  -2.626  28.579  1.00 34.76      C
ATOM   2932  N   PHE C   4      33.837  -2.947  27.024  1.00 31.97      C
ATOM   2933  CA  PHE C   4      34.173  -4.355  26.812  1.00 32.26      C
ATOM   2934  CB  PHE C   4      32.897  -5.193  26.632  1.00 34.22      C
ATOM   2935  CG  PHE C   4      32.006  -5.235  27.852  1.00 37.02      C
ATOM   2936  CD1 PHE C   4      32.481  -4.835  29.103  1.00 38.53      C
ATOM   2937  CD2 PHE C   4      30.701  -5.726  27.756  1.00 40.29      C
ATOM   2938  CE1 PHE C   4      31.673  -4.925  30.248  1.00 40.80      C
ATOM   2939  CE2 PHE C   4      29.878  -5.824  28.891  1.00 41.19      C
ATOM   2940  CZ  PHE C   4      30.369  -5.421  30.142  1.00 40.74      C
ATOM   2941  C   PHE C   4      35.052  -4.483  25.571  1.00 29.17      C
ATOM   2942  O   PHE C   4      34.655  -4.072  24.482  1.00 30.93      C
ATOM   2943  N   PRO C   5      36.257  -5.059  25.715  1.00 26.63      C
ATOM   2944  CD  PRO C   5      36.936  -5.421  26.974  1.00 24.97      C
ATOM   2945  CA  PRO C   5      37.168  -5.217  24.577  1.00 23.69      C
ATOM   2946  CB  PRO C   5      38.527  -5.052  25.227  1.00 23.66      C
ATOM   2947  CG  PRO C   5      38.335  -5.832  26.504  1.00 23.13      C
ATOM   2948  C   PRO C   5      37.043  -6.569  23.887  1.00 22.95      C
ATOM   2949  O   PRO C   5      36.403  -7.475  24.404  1.00 22.96      C
ATOM   2950  N   GLN C   6      37.666  -6.696  22.719  1.00 23.53      C
ATOM   2951  CA  GLN C   6      37.659  -7.945  21.967  1.00 21.10      C
ATOM   2952  CB  GLN C   6      37.506  -7.670  20.475  1.00 20.90      C
ATOM   2953  CG  GLN C   6      36.170  -7.105  20.063  1.00 21.10      C
ATOM   2954  CD  GLN C   6      36.074  -6.901  18.557  1.00 22.85      C
ATOM   2955  OE1 GLN C   6      36.483  -7.760  17.773  1.00 23.94      C
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| ATOM | 2956 | NE2 | GLN | C | 6 | 35.525 | -5.766 | 18.149 | 1.00 | 20.70 | C |
|------|------|-----|-----|---|---|--------|--------|--------|------|-------|---|
| ATOM | 2957 | C | GLN | C | 6 | 38.996 | -8.637 | 22.204 | 1.00 | 20.71 | C |
| ATOM | 2958 | O | GLN | C | 6 | 40.046 | -8.008 | 22.105 | 1.00 | 19.85 | C |
| ATOM | 2959 | N | PRO | C | 7 | 38.974 | -9.932 | 22.548 | 1.00 | 21.37 | C |
| ATOM | 2960 | CD | PRO | C | 7 | 37.810 | -10.710 | 23.017 | 1.00 | 21.21 | C |
| ATOM | 2961 | CA | PRO | C | 7 | 40.215 | -10.673 | 22.790 | 1.00 | 21.62 | C |
| ATOM | 2962 | CB | PRO | C | 7 | 39.783 | -11.730 | 23.795 | 1.00 | 21.96 | C |
| ATOM | 2963 | CG | PRO | C | 7 | 38.416 | -12.085 | 23.297 | 1.00 | 20.65 | C |
| ATOM | 2964 | C | PRO | C | 7 | 40.741 | -11.316 | 21.511 | 1.00 | 24.05 | C |
| ATOM | 2965 | O | PRO | C | 7 | 39.972 | -11.577 | 20.588 | 1.00 | 22.84 | C |
| ATOM | 2966 | N | GLU | C | 8 | 42.051 | -11.550 | 21.448 | 1.00 | 26.22 | C |
| ATOM | 2967 | CA | GLU | C | 8 | 42.631 | -12.215 | 20.292 | 1.00 | 27.00 | C |
| ATOM | 2968 | CB | GLU | C | 8 | 44.038 | -11.687 | 19.988 | 1.00 | 27.94 | C |
| ATOM | 2969 | CG | GLU | C | 8 | 44.803 | -12.494 | 18.915 | 1.00 | 28.38 | C |
| ATOM | 2970 | CD | GLU | C | 8 | 44.043 | -12.649 | 17.589 | 1.00 | 31.32 | C |
| ATOM | 2971 | OE1 | GLU | C | 8 | 42.980 | -13.309 | 17.564 | 1.00 | 31.69 | C |
| ATOM | 2972 | OE2 | GLU | C | 8 | 44.514 | -12.112 | 16.563 | 1.00 | 29.86 | C |
| ATOM | 2973 | C | GLU | C | 8 | 42.678 | -13.691 | 20.676 | 1.00 | 28.48 | C |
| ATOM | 2974 | O | GLU | C | 8 | 42.937 | -14.029 | 21.829 | 1.00 | 28.74 | C |
| ATOM | 2975 | N | LEU | C | 9 | 42.407 | -14.571 | 19.721 | 1.00 | 30.08 | C |
| ATOM | 2976 | CA | LEU | C | 9 | 42.404 | -15.998 | 20.002 | 1.00 | 31.21 | C |
| ATOM | 2977 | CB | LEU | C | 9 | 41.313 | -16.688 | 19.183 | 1.00 | 32.12 | C |
| ATOM | 2978 | CG | LEU | C | 9 | 39.918 | -16.072 | 19.302 | 1.00 | 33.78 | C |
| ATOM | 2979 | CD1 | LEU | C | 9 | 38.941 | -16.866 | 18.457 | 1.00 | 35.00 | C |
| ATOM | 2980 | CD2 | LEU | C | 9 | 39.481 | -16.061 | 20.761 | 1.00 | 35.59 | C |
| ATOM | 2981 | C | LEU | C | 9 | 43.748 | -16.641 | 19.712 | 1.00 | 31.83 | C |
| ATOM | 2982 | O | LEU | C | 9 | 44.342 | -16.415 | 18.658 | 1.00 | 30.94 | C |
| ATOM | 2983 | N | PRO | C | 10 | 44.256 | -17.442 | 20.657 | 1.00 | 33.31 | C |
| ATOM | 2984 | CD | PRO | C | 10 | 43.774 | -17.661 | 22.032 | 1.00 | 33.12 | C |
| ATOM | 2985 | CA | PRO | C | 10 | 45.545 | -18.097 | 20.439 | 1.00 | 36.08 | C |
| ATOM | 2986 | CB | PRO | C | 10 | 45.926 | -18.590 | 21.836 | 1.00 | 36.62 | C |
| ATOM | 2987 | CG | PRO | C | 10 | 44.598 | -18.846 | 22.476 | 1.00 | 35.26 | C |
| ATOM | 2988 | C | PRO | C | 10 | 45.428 | -19.229 | 19.430 | 1.00 | 37.51 | C |
| ATOM | 2989 | O | PRO | C | 10 | 44.495 | -20.030 | 19.491 | 1.00 | 39.49 | C |
| ATOM | 2990 | N | TYR | C | 11 | 46.365 | -19.269 | 18.488 | 1.00 | 38.68 | C |
| ATOM | 2991 | CA | TYR | C | 11 | 46.392 | -20.305 | 17.463 | 1.00 | 40.24 | C |
| ATOM | 2992 | C | TYR | C | 11 | 47.834 | -20.782 | 17.290 | 1.00 | 42.03 | C |
| ATOM | 2993 | O | TYR | C | 11 | 48.121 | -21.967 | 17.586 | 1.00 | 42.72 | C |
| ATOM | 2994 | OXT | TYR | C | 11 | 48.665 | -19.949 | 16.870 | 1.00 | 42.75 | C |
| ATOM | 2995 | CB | VAL | D | 2 | 76.722 | 40.050 | 4.030 | 1.00 | 35.81 | D |
| ATOM | 2996 | CG1 | VAL | D | 2 | 77.537 | 40.465 | 2.823 | 1.00 | 36.64 | D |
| ATOM | 2997 | CG2 | VAL | D | 2 | 76.313 | 38.577 | 3.893 | 1.00 | 37.71 | D |
| ATOM | 2998 | C | VAL | D | 2 | 76.622 | 40.298 | 6.537 | 1.00 | 31.61 | D |
| ATOM | 2999 | O | VAL | D | 2 | 75.696 | 39.494 | 6.653 | 1.00 | 31.96 | D |
| ATOM | 3000 | N | VAL | D | 2 | 78.625 | 39.207 | 5.418 | 1.00 | 32.12 | D |
| ATOM | 3001 | CA | VAL | D | 2 | 77.560 | 40.255 | 5.317 | 1.00 | 33.74 | D |
| ATOM | 3002 | N | ALA | D | 3 | 76.864 | 41.246 | 7.441 | 1.00 | 29.52 | D |
| ATOM | 3003 | CA | ALA | D | 3 | 76.053 | 41.379 | 8.653 | 1.00 | 27.92 | D |
| ATOM | 3004 | CB | ALA | D | 3 | 76.480 | 40.321 | 9.684 | 1.00 | 27.11 | D |
| ATOM | 3005 | C | ALA | D | 3 | 76.128 | 42.767 | 9.286 | 1.00 | 25.71 | D |
| ATOM | 3006 | O | ALA | D | 3 | 77.050 | 43.540 | 9.016 | 1.00 | 23.11 | D |
| ATOM | 3007 | N | ASP | D | 4 | 75.152 | 43.070 | 10.137 | 1.00 | 24.26 | D |
| ATOM | 3008 | CA | ASP | D | 4 | 75.109 | 44.354 | 10.825 | 1.00 | 24.77 | D |
| ATOM | 3009 | CB | ASP | D | 4 | 73.774 | 44.533 | 11.555 | 1.00 | 25.88 | D |
| ATOM | 3010 | CG | ASP | D | 4 | 72.595 | 44.668 | 10.611 | 1.00 | 26.24 | D |
| ATOM | 3011 | OD1 | ASP | D | 4 | 71.449 | 44.489 | 11.080 | 1.00 | 24.74 | D |
| ATOM | 3012 | OD2 | ASP | D | 4 | 72.811 | 44.961 | 9.416 | 1.00 | 28.25 | D |
| ATOM | 3013 | C | ASP | D | 4 | 76.230 | 44.407 | 11.857 | 1.00 | 25.96 | D |
| ATOM | 3014 | O | ASP | D | 4 | 76.882 | 45.437 | 12.027 | 1.00 | 26.40 | D |
| ATOM | 3015 | N | HIS | D | 5 | 76.440 | 43.290 | 12.549 | 1.00 | 24.52 | D |
| ATOM | 3016 | CA | HIS | D | 5 | 77.469 | 43.204 | 13.582 | 1.00 | 24.25 | D |
| ATOM | 3017 | CB | HIS | D | 5 | 76.836 | 43.302 | 14.972 | 1.00 | 23.42 | D |
| ATOM | 3018 | CG | HIS | D | 5 | 76.138 | 44.599 | 15.231 | 1.00 | 26.12 | D |
| ATOM | 3019 | CD2 | HIS | D | 5 | 76.567 | 45.879 | 15.126 | 1.00 | 26.16 | D |
| ATOM | 3020 | ND1 | HIS | D | 5 | 74.830 | 44.667 | 15.657 | 1.00 | 25.67 | D |
| ATOM | 3021 | CE1 | HIS | D | 5 | 74.481 | 45.932 | 15.799 | 1.00 | 26.53 | D |
| ATOM | 3022 | NE2 | HIS | D | 5 | 75.516 | 46.688 | 15.484 | 1.00 | 25.96 | D |
| ATOM | 3023 | C | HIS | D | 5 | 78.241 | 41.895 | 13.492 | 1.00 | 22.88 | D |
| ATOM | 3024 | O | HIS | D | 5 | 77.657 | 40.835 | 13.258 | 1.00 | 22.31 | D |
| ATOM | 3025 | N | VAL | D | 6 | 79.552 | 41.980 | 13.691 | 1.00 | 20.27 | D |
| ATOM | 3026 | CA | VAL | D | 6 | 80.421 | 40.815 | 13.657 | 1.00 | 19.49 | D |
| ATOM | 3027 | CB | VAL | D | 6 | 81.419 | 40.866 | 12.486 | 1.00 | 20.45 | D |
| ATOM | 3028 | CG1 | VAL | D | 6 | 82.357 | 39.674 | 12.564 | 1.00 | 19.85 | D |
| ATOM | 3029 | CG2 | VAL | D | 6 | 80.674 | 40.869 | 11.161 | 1.00 | 25.29 | D |

| ATOM | 3030 | C | VAL | D | 6 | 81.223 | 40.792 | 14.944 | 1.00 | 18.77 | D |
|------|------|------|------|---|----|---------|---------|---------|------|-------|---|
| ATOM | 3031 | O | VAL | D | 6 | 81.767 | 41.812 | 15.352 | 1.00 | 17.70 | D |
| ATOM | 3032 | N | ALA | D | 7 | 81.304 | 39.626 | 15.575 | 1.00 | 18.23 | D |
| ATOM | 3033 | CA | ALA | D | 7 | 82.046 | 39.489 | 16.821 | 1.00 | 18.01 | D |
| ATOM | 3034 | CB | ALA | D | 7 | 81.080 | 39.452 | 18.006 | 1.00 | 17.61 | D |
| ATOM | 3035 | C | ALA | D | 7 | 82.899 | 38.239 | 16.838 | 1.00 | 17.37 | D |
| ATOM | 3036 | O | ALA | D | 7 | 82.568 | 37.242 | 16.208 | 1.00 | 19.56 | D |
| ATOM | 3037 | N | SER | D | 8 | 84.008 | 38.306 | 17.562 | 1.00 | 17.07 | D |
| ATOM | 3038 | CA | SER | D | 8 | 84.892 | 37.158 | 17.712 | 1.00 | 15.46 | D |
| ATOM | 3039 | CB | SER | D | 8 | 86.297 | 37.455 | 17.202 | 1.00 | 12.56 | D |
| ATOM | 3040 | OG | SER | D | 8 | 86.324 | 37.492 | 15.789 | 1.00 | 18.97 | D |
| ATOM | 3041 | C | SER | D | 8 | 84.932 | 36.904 | 19.201 | 1.00 | 16.39 | D |
| ATOM | 3042 | O | SER | D | 8 | 85.613 | 37.614 | 19.951 | 1.00 | 15.61 | D |
| ATOM | 3043 | N | TYR | D | 9 | 84.144 | 35.930 | 19.637 | 1.00 | 17.58 | D |
| ATOM | 3044 | CA | TYR | D | 9 | 84.096 | 35.587 | 21.044 | 1.00 | 18.51 | D |
| ATOM | 3045 | CB | TYR | D | 9 | 82.698 | 35.133 | 21.444 | 1.00 | 17.92 | D |
| ATOM | 3046 | CG | TYR | D | 9 | 81.730 | 36.290 | 21.362 | 1.00 | 17.41 | D |
| ATOM | 3047 | CD1 | TYR | D | 9 | 82.056 | 37.523 | 21.928 | 1.00 | 16.27 | D |
| ATOM | 3048 | CE1 | TYR | D | 9 | 81.208 | 38.603 | 21.840 | 1.00 | 15.18 | D |
| ATOM | 3049 | CD2 | TYR | D | 9 | 80.515 | 36.169 | 20.701 | 1.00 | 17.05 | D |
| ATOM | 3050 | CE2 | TYR | D | 9 | 79.649 | 37.252 | 20.608 | 1.00 | 18.01 | D |
| ATOM | 3051 | CZ | TYR | D | 9 | 80.005 | 38.466 | 21.181 | 1.00 | 16.67 | D |
| ATOM | 3052 | OH | TYR | D | 9 | 79.157 | 39.543 | 21.104 | 1.00 | 20.30 | D |
| ATOM | 3053 | C | TYR | D | 9 | 85.120 | 34.508 | 21.115 | 1.00 | 19.92 | D |
| ATOM | 3054 | O | TYR | D | 9 | 84.856 | 33.323 | 21.337 | 1.00 | 17.21 | D |
| ATOM | 3055 | N | GLY | D | 10 | 86.321 | 34.989 | 20.843 | 1.00 | 22.61 | D |
| ATOM | 3056 | CA | GLY | D | 10 | 87.478 | 34.160 | 20.836 | 1.00 | 20.96 | D |
| ATOM | 3057 | C | GLY | D | 10 | 88.358 | 34.354 | 19.624 | 1.00 | 18.79 | D |
| ATOM | 3058 | O | GLY | D | 10 | 88.170 | 33.693 | 18.618 | 1.00 | 16.79 | D |
| ATOM | 3059 | N | VAL | D | 11 | 89.275 | 35.307 | 19.683 | 1.00 | 17.75 | D |
| ATOM | 3060 | CA | VAL | D | 11 | 90.256 | 35.394 | 18.616 | 1.00 | 16.92 | D |
| ATOM | 3061 | CB | VAL | D | 11 | 90.666 | 36.829 | 18.242 | 1.00 | 17.76 | D |
| ATOM | 3062 | CG1 | VAL | D | 11 | 91.873 | 36.778 | 17.313 | 1.00 | 15.46 | D |
| ATOM | 3063 | CG2 | VAL | D | 11 | 89.522 | 37.544 | 17.544 | 1.00 | 13.00 | D |
| ATOM | 3064 | C | VAL | D | 11 | 91.391 | 34.728 | 19.395 | 1.00 | 17.46 | D |
| ATOM | 3065 | O | VAL | D | 11 | 91.865 | 35.266 | 20.405 | 1.00 | 18.93 | D |
| ATOM | 3066 | N | ASN | D | 12 | 91.773 | 33.531 | 18.973 | 1.00 | 17.46 | D |
| ATOM | 3067 | CA | ASN | D | 12 | 92.831 | 32.779 | 19.644 | 1.00 | 18.01 | D |
| ATOM | 3068 | CB | ASN | D | 12 | 92.339 | 31.360 | 19.969 | 1.00 | 16.68 | D |
| ATOM | 3069 | CG | ASN | D | 12 | 91.179 | 31.356 | 20.955 | 1.00 | 16.27 | D |
| ATOM | 3070 | OD1 | ASN | D | 12 | 91.346 | 30.989 | 22.115 | 1.00 | 14.97 | D |
| ATOM | 3071 | ND2 | ASN | D | 12 | 90.000 | 31.779 | 20.497 | 1.00 | 14.97 | D |
| ATOM | 3072 | C | ASN | D | 12 | 94.061 | 32.699 | 18.759 | 1.00 | 18.74 | D |
| ATOM | 3073 | O | ASN | D | 12 | 93.963 | 32.373 | 17.578 | 1.00 | 19.66 | D |
| ATOM | 3074 | N | LEU | D | 13 | 95.221 | 32.969 | 19.344 | 1.00 | 20.75 | D |
| ATOM | 3075 | CA | LEU | D | 13 | 96.471 | 32.949 | 18.600 | 1.00 | 22.59 | D |
| ATOM | 3076 | CB | LEU | D | 13 | 96.841 | 34.387 | 18.234 | 1.00 | 24.32 | D |
| ATOM | 3077 | CG | LEU | D | 13 | 98.215 | 34.672 | 17.632 | 1.00 | 25.29 | D |
| ATOM | 3078 | CD1 | LEU | D | 13 | 98.355 | 33.966 | 16.289 | 1.00 | 24.58 | D |
| ATOM | 3079 | CD2 | LEU | D | 13 | 98.380 | 36.177 | 17.475 | 1.00 | 23.52 | D |
| ATOM | 3080 | C | LEU | D | 13 | 97.646 | 32.290 | 19.330 | 1.00 | 22.44 | D |
| ATOM | 3081 | O | LEU | D | 13 | 97.900 | 32.578 | 20.494 | 1.00 | 24.67 | D |
| ATOM | 3082 | N | TYR | D | 14 | 98.350 | 31.397 | 18.641 | 1.00 | 23.69 | D |
| ATOM | 3083 | CA | TYR | D | 14 | 99.535 | 30.740 | 19.196 | 1.00 | 25.57 | D |
| ATOM | 3084 | CB | TYR | D | 14 | 99.223 | 29.360 | 19.765 | 1.00 | 26.53 | D |
| ATOM | 3085 | CG | TYR | D | 14 | 100.445 | 28.712 | 20.383 | 1.00 | 28.87 | D |
| ATOM | 3086 | CD1 | TYR | D | 14 | 100.872 | 29.057 | 21.668 | 1.00 | 28.57 | D |
| ATOM | 3087 | CE1 | TYR | D | 14 | 102.032 | 28.500 | 22.218 | 1.00 | 27.29 | D |
| ATOM | 3088 | CD2 | TYR | D | 14 | 101.209 | 27.793 | 19.664 | 1.00 | 29.65 | D |
| ATOM | 3089 | CE2 | TYR | D | 14 | 102.369 | 27.235 | 20.204 | 1.00 | 26.94 | D |
| ATOM | 3090 | CZ | TYR | D | 14 | 102.773 | 27.592 | 21.477 | 1.00 | 27.22 | D |
| ATOM | 3091 | OH | TYR | D | 14 | 103.914 | 27.039 | 22.008 | 1.00 | 29.69 | D |
| ATOM | 3092 | C | TYR | D | 14 | 100.553 | 30.574 | 18.074 | 1.00 | 26.73 | D |
| ATOM | 3093 | O | TYR | D | 14 | 100.210 | 30.128 | 16.980 | 1.00 | 27.22 | D |
| ATOM | 3094 | N | GLN | D | 15 | 101.800 | 30.945 | 18.338 | 1.00 | 26.92 | D |
| ATOM | 3095 | CA | GLN | D | 15 | 102.847 | 30.820 | 17.332 | 1.00 | 27.70 | D |
| ATOM | 3096 | CB | GLN | D | 15 | 103.164 | 32.179 | 16.710 | 1.00 | 27.39 | D |
| ATOM | 3097 | CG | GLN | D | 15 | 103.534 | 33.251 | 17.704 | 1.00 | 27.78 | D |
| ATOM | 3098 | CD | GLN | D | 15 | 103.806 | 34.590 | 17.044 | 1.00 | 27.70 | D |
| ATOM | 3099 | OE1 | GLN | D | 15 | 103.723 | 35.638 | 17.685 | 1.00 | 31.07 | D |
| ATOM | 3100 | NE2 | GLN | D | 15 | 104.142 | 34.562 | 15.763 | 1.00 | 25.83 | D |
| ATOM | 3101 | C | GLN | D | 15 | 104.097 | 30.222 | 17.952 | 1.00 | 28.40 | D |
| ATOM | 3102 | O | GLN | D | 15 | 104.368 | 30.416 | 19.141 | 1.00 | 28.81 | D |
| ATOM | 3103 | N | SER | D | 16 | 104.852 | 29.488 | 17.143 | 1.00 | 27.95 | D |

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| ATOM | 3104 | CA | SER | D | 16 | 106.070 | 28.834 | 17.611 | 1.00 | 28.04 | D |
| ATOM | 3105 | CB | SER | D | 16 | 106.613 | 27.887 | 16.534 | 1.00 | 25.04 | D |
| ATOM | 3106 | OG | SER | D | 16 | 106.879 | 28.581 | 15.330 | 1.00 | 26.28 | D |
| ATOM | 3107 | C | SER | D | 16 | 107.155 | 29.824 | 18.024 | 1.00 | 27.77 | D |
| ATOM | 3108 | O | SER | D | 16 | 107.922 | 29.558 | 18.946 | 1.00 | 26.81 | D |
| ATOM | 3109 | N | TYR | D | 17 | 107.221 | 30.965 | 17.351 | 1.00 | 29.70 | D |
| ATOM | 3110 | CA | TYR | D | 17 | 108.228 | 31.953 | 17.694 | 1.00 | 32.41 | D |
| ATOM | 3111 | CB | TYR | D | 17 | 108.248 | 33.086 | 16.672 | 1.00 | 35.15 | D |
| ATOM | 3112 | CG | TYR | D | 17 | 109.440 | 33.986 | 16.864 | 1.00 | 40.80 | D |
| ATOM | 3113 | CD1 | TYR | D | 17 | 110.719 | 33.556 | 16.508 | 1.00 | 43.28 | D |
| ATOM | 3114 | CE1 | TYR | D | 17 | 111.836 | 34.345 | 16.743 | 1.00 | 44.62 | D |
| ATOM | 3115 | CD2 | TYR | D | 17 | 109.308 | 35.235 | 17.460 | 1.00 | 40.97 | D |
| ATOM | 3116 | CE2 | TYR | D | 17 | 110.419 | 36.032 | 17.702 | 1.00 | 44.83 | D |
| ATOM | 3117 | CZ | TYR | D | 17 | 111.679 | 35.580 | 17.341 | 1.00 | 45.74 | D |
| ATOM | 3118 | OH | TYR | D | 17 | 112.788 | 36.353 | 17.590 | 1.00 | 49.39 | D |
| ATOM | 3119 | C | TYR | D | 17 | 107.954 | 32.525 | 19.084 | 1.00 | 33.13 | D |
| ATOM | 3120 | O | TYR | D | 17 | 106.888 | 33.092 | 19.332 | 1.00 | 32.77 | D |
| ATOM | 3121 | N | GLY | D | 18 | 108.930 | 32.383 | 19.981 | 1.00 | 32.74 | D |
| ATOM | 3122 | CA | GLY | D | 18 | 108.780 | 32.867 | 21.341 | 1.00 | 31.76 | D |
| ATOM | 3123 | C | GLY | D | 18 | 108.958 | 31.716 | 22.311 | 1.00 | 32.63 | D |
| ATOM | 3124 | O | GLY | D | 18 | 110.005 | 31.600 | 22.948 | 1.00 | 34.20 | D |
| ATOM | 3125 | N | PRO | D | 19 | 107.946 | 30.840 | 22.452 | 1.00 | 33.13 | D |
| ATOM | 3126 | CD | PRO | D | 19 | 108.029 | 29.606 | 23.256 | 1.00 | 31.73 | D |
| ATOM | 3127 | CA | PRO | D | 19 | 106.663 | 30.906 | 21.741 | 1.00 | 32.71 | D |
| ATOM | 3128 | CB | PRO | D | 19 | 106.115 | 29.492 | 21.903 | 1.00 | 33.20 | D |
| ATOM | 3129 | CG | PRO | D | 19 | 106.591 | 29.128 | 23.280 | 1.00 | 31.76 | D |
| ATOM | 3130 | C | PRO | D | 19 | 105.768 | 31.948 | 22.406 | 1.00 | 32.52 | D |
| ATOM | 3131 | O | PRO | D | 19 | 105.970 | 32.282 | 23.568 | 1.00 | 33.11 | D |
| ATOM | 3132 | N | SER | D | 20 | 104.786 | 32.463 | 21.676 | 1.00 | 31.92 | D |
| ATOM | 3133 | CA | SER | D | 20 | 103.886 | 33.455 | 22.246 | 1.00 | 30.99 | D |
| ATOM | 3134 | CB | SER | D | 20 | 104.287 | 34.867 | 21.795 | 1.00 | 30.92 | D |
| ATOM | 3135 | OG | SER | D | 20 | 104.263 | 34.988 | 20.381 | 1.00 | 33.16 | D |
| ATOM | 3136 | C | SER | D | 20 | 102.441 | 33.172 | 21.852 | 1.00 | 30.01 | D |
| ATOM | 3137 | O | SER | D | 20 | 102.179 | 32.428 | 20.902 | 1.00 | 29.42 | D |
| ATOM | 3138 | N | GLY | D | 21 | 101.512 | 33.763 | 22.598 | 1.00 | 27.60 | D |
| ATOM | 3139 | CA | GLY | D | 21 | 100.101 | 33.580 | 22.318 | 1.00 | 25.70 | D |
| ATOM | 3140 | C | GLY | D | 21 | 99.309 | 34.836 | 22.632 | 1.00 | 24.66 | D |
| ATOM | 3141 | O | GLY | D | 21 | 99.848 | 35.798 | 23.187 | 1.00 | 23.84 | D |
| ATOM | 3142 | N | GLN | D | 22 | 98.030 | 34.834 | 22.268 | 1.00 | 22.55 | D |
| ATOM | 3143 | CA | GLN | D | 22 | 97.149 | 35.974 | 22.527 | 1.00 | 20.16 | D |
| ATOM | 3144 | CB | GLN | D | 22 | 97.301 | 37.049 | 21.445 | 1.00 | 18.28 | D |
| ATOM | 3145 | CG | GLN | D | 22 | 96.416 | 38.284 | 21.672 | 1.00 | 18.60 | D |
| ATOM | 3146 | CD | GLN | D | 22 | 96.513 | 39.327 | 20.562 | 1.00 | 18.36 | D |
| ATOM | 3147 | OE1 | GLN | D | 22 | 97.379 | 40.207 | 20.587 | 1.00 | 19.82 | D |
| ATOM | 3148 | NE2 | GLN | D | 22 | 95.617 | 39.232 | 19.582 | 1.00 | 17.69 | D |
| ATOM | 3149 | C | GLN | D | 22 | 95.699 | 35.517 | 22.561 | 1.00 | 18.61 | D |
| ATOM | 3150 | O | GLN | D | 22 | 95.301 | 34.638 | 21.790 | 1.00 | 17.26 | D |
| ATOM | 3151 | N | TYR | D | 23 | 94.926 | 36.097 | 23.475 | 1.00 | 16.42 | D |
| ATOM | 3152 | CA | TYR | D | 23 | 93.507 | 35.785 | 23.592 | 1.00 | 16.21 | D |
| ATOM | 3153 | CB | TYR | D | 23 | 93.212 | 34.839 | 24.762 | 1.00 | 14.97 | D |
| ATOM | 3154 | CG | TYR | D | 23 | 91.750 | 34.438 | 24.798 | 1.00 | 14.24 | D |
| ATOM | 3155 | CD1 | TYR | D | 23 | 91.309 | 33.318 | 24.109 | 1.00 | 14.49 | D |
| ATOM | 3156 | CE1 | TYR | D | 23 | 89.969 | 33.004 | 24.029 | 1.00 | 14.23 | D |
| ATOM | 3157 | CD2 | TYR | D | 23 | 90.795 | 35.240 | 25.421 | 1.00 | 13.21 | D |
| ATOM | 3158 | CE2 | TYR | D | 23 | 89.443 | 34.934 | 25.344 | 1.00 | 13.08 | D |
| ATOM | 3159 | CZ | TYR | D | 23 | 89.039 | 33.814 | 24.647 | 1.00 | 12.88 | D |
| ATOM | 3160 | OH | TYR | D | 23 | 87.710 | 33.471 | 24.566 | 1.00 | 16.44 | D |
| ATOM | 3161 | C | TYR | D | 23 | 92.751 | 37.089 | 23.806 | 1.00 | 15.56 | D |
| ATOM | 3162 | O | TYR | D | 23 | 93.014 | 37.817 | 24.763 | 1.00 | 16.57 | D |
| ATOM | 3163 | N | THR | D | 24 | 91.811 | 37.377 | 22.914 | 1.00 | 14.11 | D |
| ATOM | 3164 | CA | THR | D | 24 | 91.026 | 38.598 | 22.995 | 1.00 | 13.31 | D |
| ATOM | 3165 | CB | THR | D | 24 | 91.606 | 39.692 | 22.071 | 1.00 | 16.07 | D |
| ATOM | 3166 | OG1 | THR | D | 24 | 91.682 | 39.176 | 20.734 | 1.00 | 17.94 | D |
| ATOM | 3167 | CG2 | THR | D | 24 | 92.992 | 40.116 | 22.514 | 1.00 | 13.19 | D |
| ATOM | 3168 | C | THR | D | 24 | 89.604 | 38.342 | 22.519 | 1.00 | 12.68 | D |
| ATOM | 3169 | O | THR | D | 24 | 89.306 | 37.287 | 21.994 | 1.00 | 15.13 | D |
| ATOM | 3170 | N | HIS | D | 25 | 88.726 | 39.312 | 22.727 | 1.00 | 13.47 | D |
| ATOM | 3171 | CA | HIS | D | 25 | 87.360 | 39.224 | 22.229 | 1.00 | 13.83 | D |
| ATOM | 3172 | CB | HIS | D | 25 | 86.326 | 39.132 | 23.346 | 1.00 | 11.26 | D |
| ATOM | 3173 | CG | HIS | D | 25 | 86.053 | 37.727 | 23.785 | 1.00 | 14.42 | D |
| ATOM | 3174 | CD2 | HIS | D | 25 | 86.815 | 36.610 | 23.723 | 1.00 | 12.09 | D |
| ATOM | 3175 | ND1 | HIS | D | 25 | 84.876 | 37.351 | 24.392 | 1.00 | 15.93 | D |
| ATOM | 3176 | CE1 | HIS | D | 25 | 84.922 | 36.064 | 24.685 | 1.00 | 14.24 | D |
| ATOM | 3177 | NE2 | HIS | D | 25 | 86.089 | 35.591 | 24.289 | 1.00 | 13.67 | D |

| ATOM | 3178 | C   | HIS D | 25 | 87.158 | 40.495 | 21.436 | 1.00 13.30 | D |
|------|------|-----|-------|----|--------|--------|--------|------------|---|
| ATOM | 3179 | O   | HIS D | 25 | 87.573 | 41.563 | 21.859 | 1.00 13.77 | D |
| ATOM | 3180 | N   | GLU D | 26 | 86.544 | 40.376 | 20.271 | 1.00 15.40 | D |
| ATOM | 3181 | CA  | GLU D | 26 | 86.318 | 41.540 | 19.434 | 1.00 16.53 | D |
| ATOM | 3182 | CB  | GLU D | 26 | 87.109 | 41.396 | 18.133 | 1.00 14.47 | D |
| ATOM | 3183 | CG  | GLU D | 26 | 88.627 | 41.460 | 18.277 | 1.00 14.81 | D |
| ATOM | 3184 | CD  | GLU D | 26 | 89.341 | 41.205 | 16.947 | 1.00 19.22 | D |
| ATOM | 3185 | OE1 | GLU D | 26 | 88.726 | 41.429 | 15.884 | 1.00 22.84 | D |
| ATOM | 3186 | OE2 | GLU D | 26 | 90.512 | 40.792 | 16.953 | 1.00 17.41 | D |
| ATOM | 3187 | C   | GLU D | 26 | 84.841 | 41.721 | 19.111 | 1.00 17.28 | D |
| ATOM | 3188 | O   | GLU D | 26 | 84.073 | 40.760 | 19.100 | 1.00 16.62 | D |
| ATOM | 3189 | N   | PHE D | 27 | 84.455 | 42.971 | 18.879 | 1.00 19.63 | D |
| ATOM | 3190 | CA  | PHE D | 27 | 83.092 | 43.313 | 18.494 | 1.00 19.71 | D |
| ATOM | 3191 | CB  | PHE D | 27 | 82.231 | 43.722 | 19.684 | 1.00 21.05 | D |
| ATOM | 3192 | CG  | PHE D | 27 | 80.758 | 43.816 | 19.348 | 1.00 24.29 | D |
| ATOM | 3193 | CD1 | PHE D | 27 | 79.971 | 42.668 | 19.278 | 1.00 23.22 | D |
| ATOM | 3194 | CD2 | PHE D | 27 | 80.169 | 45.047 | 19.073 | 1.00 22.47 | D |
| ATOM | 3195 | CE1 | PHE D | 27 | 78.617 | 42.744 | 18.940 | 1.00 24.89 | D |
| ATOM | 3196 | CE2 | PHE D | 27 | 78.818 | 45.132 | 18.733 | 1.00 24.72 | D |
| ATOM | 3197 | CZ  | PHE D | 27 | 78.041 | 43.980 | 18.667 | 1.00 22.80 | D |
| ATOM | 3198 | C   | PHE D | 27 | 83.182 | 44.482 | 17.532 | 1.00 18.41 | D |
| ATOM | 3199 | O   | PHE D | 27 | 83.700 | 45.545 | 17.879 | 1.00 19.21 | D |
| ATOM | 3200 | N   | ASP D | 28 | 82.680 | 44.272 | 16.321 | 1.00 18.46 | D |
| ATOM | 3201 | CA  | ASP D | 28 | 82.700 | 45.284 | 15.272 | 1.00 18.63 | D |
| ATOM | 3202 | CB  | ASP D | 28 | 81.702 | 46.404 | 15.568 | 1.00 19.29 | D |
| ATOM | 3203 | CG  | ASP D | 28 | 80.268 | 45.981 | 15.305 | 1.00 22.52 | D |
| ATOM | 3204 | OD1 | ASP D | 28 | 80.076 | 44.885 | 14.738 | 1.00 23.13 | D |
| ATOM | 3205 | OD2 | ASP D | 28 | 79.333 | 46.736 | 15.651 | 1.00 24.61 | D |
| ATOM | 3206 | C   | ASP D | 28 | 84.075 | 45.865 | 15.037 | 1.00 17.83 | D |
| ATOM | 3207 | O   | ASP D | 28 | 84.225 | 47.069 | 14.860 | 1.00 20.60 | D |
| ATOM | 3208 | N   | GLY D | 29 | 85.079 | 44.997 | 15.042 | 1.00 18.44 | D |
| ATOM | 3209 | CA  | GLY D | 29 | 86.439 | 45.431 | 14.788 | 1.00 19.49 | D |
| ATOM | 3210 | C   | GLY D | 29 | 87.218 | 46.011 | 15.949 | 1.00 18.93 | D |
| ATOM | 3211 | O   | GLY D | 29 | 88.382 | 46.359 | 15.784 | 1.00 19.51 | D |
| ATOM | 3212 | N   | ASP D | 30 | 86.595 | 46.122 | 17.117 | 1.00 17.91 | D |
| ATOM | 3213 | CA  | ASP D | 30 | 87.279 | 46.667 | 18.288 | 1.00 17.21 | D |
| ATOM | 3214 | CB  | ASP D | 30 | 86.499 | 47.858 | 18.831 | 1.00 15.85 | D |
| ATOM | 3215 | CG  | ASP D | 30 | 86.594 | 49.060 | 17.924 | 1.00 18.96 | D |
| ATOM | 3216 | OD1 | ASP D | 30 | 87.731 | 49.515 | 17.668 | 1.00 18.56 | D |
| ATOM | 3217 | OD2 | ASP D | 30 | 85.541 | 49.544 | 17.466 | 1.00 19.00 | D |
| ATOM | 3218 | C   | ASP D | 30 | 87.491 | 45.629 | 19.389 | 1.00 17.20 | D |
| ATOM | 3219 | O   | ASP D | 30 | 86.651 | 44.763 | 19.621 | 1.00 15.68 | D |
| ATOM | 3220 | N   | GLU D | 31 | 88.629 | 45.739 | 20.062 | 1.00 18.79 | D |
| ATOM | 3221 | CA  | GLU D | 31 | 89.015 | 44.829 | 21.131 | 1.00 17.52 | D |
| ATOM | 3222 | CB  | GLU D | 31 | 90.531 | 44.947 | 21.363 | 1.00 19.03 | D |
| ATOM | 3223 | CG  | GLU D | 31 | 91.074 | 44.215 | 22.579 | 1.00 22.08 | D |
| ATOM | 3224 | CD  | GLU D | 31 | 92.596 | 44.254 | 22.653 | 1.00 25.29 | D |
| ATOM | 3225 | OE1 | GLU D | 31 | 93.198 | 45.159 | 22.041 | 1.00 26.54 | D |
| ATOM | 3226 | OE2 | GLU D | 31 | 93.193 | 43.387 | 23.331 | 1.00 25.19 | D |
| ATOM | 3227 | C   | GLU D | 31 | 88.248 | 45.109 | 22.421 | 1.00 17.80 | D |
| ATOM | 3228 | O   | GLU D | 31 | 88.360 | 46.195 | 23.004 | 1.00 16.81 | D |
| ATOM | 3229 | N   | GLN D | 32 | 87.478 | 44.118 | 22.862 | 1.00 15.25 | D |
| ATOM | 3230 | CA  | GLN D | 32 | 86.685 | 44.230 | 24.085 | 1.00 15.53 | D |
| ATOM | 3231 | CB  | GLN D | 32 | 85.502 | 43.260 | 24.044 | 1.00 12.86 | D |
| ATOM | 3232 | CG  | GLN D | 32 | 84.391 | 43.680 | 23.101 | 1.00 13.72 | D |
| ATOM | 3233 | CD  | GLN D | 32 | 83.233 | 42.708 | 23.111 | 1.00 16.53 | D |
| ATOM | 3234 | OE1 | GLN D | 32 | 83.407 | 41.526 | 22.838 | 1.00 20.27 | D |
| ATOM | 3235 | NE2 | GLN D | 32 | 82.044 | 43.203 | 23.423 | 1.00 17.48 | D |
| ATOM | 3236 | C   | GLN D | 32 | 87.528 | 43.956 | 25.329 | 1.00 16.00 | D |
| ATOM | 3237 | O   | GLN D | 32 | 87.356 | 44.603 | 26.366 | 1.00 15.18 | D |
| ATOM | 3238 | N   | PHE D | 33 | 88.423 | 42.981 | 25.222 | 1.00 16.17 | D |
| ATOM | 3239 | CA  | PHE D | 33 | 89.315 | 42.638 | 26.321 | 1.00 15.74 | D |
| ATOM | 3240 | CB  | PHE D | 33 | 88.520 | 42.083 | 27.515 | 1.00 15.40 | D |
| ATOM | 3241 | CG  | PHE D | 33 | 87.969 | 40.693 | 27.307 | 1.00 15.83 | D |
| ATOM | 3242 | CD1 | PHE D | 33 | 88.781 | 39.572 | 27.480 | 1.00 16.23 | D |
| ATOM | 3243 | CD2 | PHE D | 33 | 86.625 | 40.503 | 26.977 | 1.00 17.27 | D |
| ATOM | 3244 | CE1 | PHE D | 33 | 88.262 | 38.282 | 27.332 | 1.00 15.79 | D |
| ATOM | 3245 | CE2 | PHE D | 33 | 86.088 | 39.218 | 26.827 | 1.00 15.20 | D |
| ATOM | 3246 | CZ  | PHE D | 33 | 86.909 | 38.108 | 27.006 | 1.00 17.77 | D |
| ATOM | 3247 | C   | PHE D | 33 | 90.330 | 41.614 | 25.860 | 1.00 15.28 | D |
| ATOM | 3248 | O   | PHE D | 33 | 90.157 | 40.979 | 24.825 | 1.00 15.16 | D |
| ATOM | 3249 | N   | TYR D | 34 | 91.405 | 41.476 | 26.620 | 1.00 15.54 | D |
| ATOM | 3250 | CA  | TYR D | 34 | 92.414 | 40.480 | 26.314 | 1.00 16.00 | D |
| ATOM | 3251 | CB  | TYR D | 34 | 93.649 | 41.124 | 25.670 | 1.00 17.46 | D |

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| ATOM | 3252 | CG | TYR D | 34 | 94.508 | 41.970 | 26.588 | 1.00 | 20.90 | D |
|------|------|-----|--------|-----|---------|---------|---------|------|-------|---|
| ATOM | 3253 | CD1 | TYR D | 34 | 95.488 | 41.390 | 27.391 | 1.00 | 21.91 | D |
| ATOM | 3254 | CE1 | TYR D | 34 | 96.295 | 42.174 | 28.221 | 1.00 | 24.17 | D |
| ATOM | 3255 | CD2 | TYR D | 34 | 94.351 | 43.354 | 26.638 | 1.00 | 20.26 | D |
| ATOM | 3256 | CE2 | TYR D | 34 | 95.147 | 44.141 | 27.463 | 1.00 | 24.97 | D |
| ATOM | 3257 | CZ | TYR D | 34 | 96.117 | 43.546 | 28.251 | 1.00 | 23.87 | D |
| ATOM | 3258 | OH | TYR D | 34 | 96.904 | 44.326 | 29.065 | 1.00 | 26.29 | D |
| ATOM | 3259 | C | TYR D | 34 | 92.766 | 39.836 | 27.642 | 1.00 | 16.56 | D |
| ATOM | 3260 | O | TYR D | 34 | 92.476 | 40.386 | 28.699 | 1.00 | 15.36 | D |
| ATOM | 3261 | N | VAL D | 35 | 93.354 | 38.653 | 27.586 | 1.00 | 18.29 | D |
| ATOM | 3262 | CA | VAL D | 35 | 93.768 | 37.971 | 28.795 | 1.00 | 19.11 | D |
| ATOM | 3263 | CB | VAL D | 35 | 93.257 | 36.514 | 28.842 | 1.00 | 17.61 | D |
| ATOM | 3264 | CG1 | VAL D | 35 | 93.910 | 35.780 | 29.992 | 1.00 | 17.99 | D |
| ATOM | 3265 | CG2 | VAL D | 35 | 91.744 | 36.493 | 29.003 | 1.00 | 17.82 | D |
| ATOM | 3266 | C | VAL D | 35 | 95.290 | 37.950 | 28.813 | 1.00 | 19.96 | D |
| ATOM | 3267 | O | VAL D | 35 | 95.914 | 37.492 | 27.866 | 1.00 | 17.73 | D |
| ATOM | 3268 | N | ASP D | 36 | 95.883 | 38.473 | 29.880 | 1.00 | 22.63 | D |
| ATOM | 3269 | CA | ASP D | 36 | 97.333 | 38.456 | 30.005 | 1.00 | 24.79 | D |
| ATOM | 3270 | CB | ASP D | 36 | 97.795 | 39.409 | 31.106 | 1.00 | 26.41 | D |
| ATOM | 3271 | CG | ASP D | ,36 | 99.298 | 39.574 | 31.131 | 1.00 | 30.12 | D |
| ATOM | 3272 | OD1 | ASP D | 36 | 100.002 | 38.547 | 31.252 | 1.00 | 32.04 | D |
| ATOM | 3273 | OD2 | ASP D | 36 | 99.776 | 40.726 | 31.028 | 1.00 | 32.20 | D |
| ATOM | 3274 | C | ASP D | 36 | 97.650 | 37.011 | 30.389 | 1.00 | 25.23 | D |
| ATOM | 3275 | O | ASP D | 36 | 97.349 | 36.575 | 31.502 | 1.00 | 25.21 | D |
| ATOM | 3276 | N | LEU D | 37 | 98.236 | 36.272 | 29.455 | 1.00 | 23.64 | D |
| ATOM | 3277 | CA | LEU D | 37 | 98.549 | 34.870 | 29.676 | 1.00 | 25.25 | D |
| ATOM | 3278 | CB | LEU D | 37 | 98.992 | 34.232 | 28.355 | 1.00 | 21.08 | D |
| ATOM | 3279 | CG | LEU D | 37 | 97.955 | 34.360 | 27.225 | 1.00 | 20.24 | D |
| ATOM | 3280 | CD1 | LEU D | 37 | 98.568 | 33.934 | 25.899 | 1.00 | 17.23 | D |
| ATOM | 3281 | CD2 | LEU D | 37 | 96.730 | 33.516 | 27.541 | 1.00 | 19.11 | D |
| ATOM | 3282 | C | LEU D | 37 | 99.590 | 34.626 | 30.770 | 1.00 | 27.73 | D |
| ATOM | 3283 | O | LEU D | 37 | 99.464 | 33.682 | 31.554 | 1.00 | 27.92 | D |
| ATOM | 3284 | N | GLY D | 38 | 100.608 | 35.474 | 30.837 | 1.00 | 29.31 | D |
| ATOM | 3285 | CA | GLY D | 38 | 101.629 | 35.292 | 31.851 | 1.00 | 30.44 | D |
| ATOM | 3286 | C | GLY D | 38 | 101.141 | 35.640 | 33.242 | 1.00 | 32.52 | D |
| ATOM | 3287 | O | GLY D | 38 | 101.502 | 34.986 | 34.220 | 1.00 | 34.37 | D |
| ATOM | 3288 | N | ARG D | 39 | 100.309 | 36.669 | 33.335 | 1.00 | 35.10 | D |
| ATOM | 3289 | CA | ARG D | 39 | 99.786 | 37.103 | 34.623 | 1.00 | 36.92 | D |
| ATOM | 3290 | CB | ARG D | 39 | 99.693 | 38.632 | 34.653 | 1.00 | 39.96 | D |
| ATOM | 3291 | CG | ARG D | 39 | 101.011 | 39.318 | 34.301 | 1.00 | 44.57 | D |
| ATOM | 3292 | CD | ARG D | 39 | 101.006 | 40.798 | 34.667 | 1.00 | 49.71 | D |
| ATOM | 3293 | NE | ARG D | 39 | 102.240 | 41.484 | 34.270 | 1.00 | 53.08 | D |
| ATOM | 3294 | CZ | ARG D | 39 | 103.460 | 41.164 | 34.698 | 1.00 | 55.33 | D |
| ATOM | 3295 | NH1 | ARG D | 39 | 103.635 | 40.158 | 35.546 | 1.00 | 56.98 | D |
| ATOM | 3296 | NH2 | ARG D | 39 | 104.512 | 41.859 | 34.282 | 1.00 | 56.80 | D |
| ATOM | 3297 | C | ARG D | 39 | 98.429 | 36.476 | 34.924 | 1.00 | 35.86 | D |
| ATOM | 3298 | O | ARG D | 39 | 97.886 | 36.630 | 36.022 | 1.00 | 35.27 | D |
| ATOM | 3299 | N | LYS D | 40 | 97.893 | 35.757 | 33.944 | 1.00 | 34.51 | D |
| ATOM | 3300 | CA | LYS D | 40 | 96.602 | 35.095 | 34.090 | 1.00 | 33.49 | D |
| ATOM | 3301 | CB | LYS D | 40 | 96.714 | 33.939 | 35.088 | 1.00 | 34.77 | D |
| ATOM | 3302 | CG | LYS D | 40 | 95.482 | 33.040 | 35.133 | 1.00 | 41.38 | D |
| ATOM | 3303 | CD | LYS D | 40 | 95.703 | 31.839 | 36.046 | 1.00 | 45.02 | D |
| ATOM | 3304 | CE | LYS D | 40 | 94.443 | 31.001 | 36.185 | 1.00 | 46.54 | D |
| ATOM | 3305 | NZ | LYS D | 40 | 94.652 | 29.853 | 37.112 | 1.00 | 48.98 | D |
| ATOM | 3306 | C | LYS D | 40 | 95.511 | 36.064 | 34.542 | 1.00 | 30.95 | D |
| ATOM | 3307 | O | LYS D | 40 | 94.780 | 35.794 | 35.492 | 1.00 | 28.23 | D |
| ATOM | 3308 | N | GLU D | 41 | 95.401 | 37.197 | 33.858 | 1.00 | 30.54 | D |
| ATOM | 3309 | CA | GLU D | 41 | 94.384 | 38.175 | 34.210 | 1.00 | 30.41 | D |
| ATOM | 3310 | CB | GLU D | 41 | 94.980 | 39.302 | 35.078 | 1.00 | 34.10 | D |
| ATOM | 3311 | CG | GLU D | 41 | 96.180 | 40.034 | 34.488 | 1.00 | 41.52 | D |
| ATOM | 3312 | CD | GLU D | 41 | 96.834 | 40.997 | 35.482 | 1.00 | 45.72 | D |
| ATOM | 3313 | OE1 | GLU D | 41 | 97.826 | 41.665 | 35.108 | 1.00 | 48.68 | D |
| ATOM | 3314 | OE2 | GLU D | 41 | 96.362 | 41.086 | 36.638 | 1.00 | 47.60 | D |
| ATOM | 3315 | C | GLU D | 41 | 93.651 | 38.766 | 33.014 | 1.00 | 28.03 | D |
| ATOM | 3316 | O | GLU D | 41 | 94.220 | 38.981 | 31.940 | 1.00 | 25.49 | D |
| ATOM | 3317 | N | THR D | 42 | 92.364 | 39.006 | 33.226 | 1.00 | 25.48 | D |
| ATOM | 3318 | CA | THR D | 42 | 91.488 | 39.582 | 32.224 | 1.00 | 23.42 | D |
| ATOM | 3319 | CB | THR D | 42 | 90.035 | 39.187 | 32.511 | 1.00 | 22.07 | D |
| ATOM | 3320 | OG1 | THR D | 42 | 89.927 | 37.761 | 32.468 | 1.00 | 18.54 | D |
| ATOM | 3321 | CG2 | THR D | 42 | 89.087 | 39.817 | 31.497 | 1.00 | 20.32 | D |
| ATOM | 3322 | C | THR D | 42 | 91.615 | 41.098 | 32.301 | 1.00 | 22.29 | D |
| ATOM | 3323 | O | THR D | 42 | 91.492 | 41.680 | 33.373 | 1.00 | 21.54 | D |
| ATOM | 3324 | N | VAL D | 43 | 91.874 | 41.736 | 31.167 | 1.00 | 21.50 | D |
| ATOM | 3325 | CA | VAL D | 43 | 92.004 | 43.183 | 31.136 | 1.00 | 19.88 | D |

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| ATOM | 3326 | CB | VAL | D | 43 | 93.428 | 43.584 | 30.697 | 1.00 | 21.56 | D |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 3327 | CG1 | VAL | D | 43 | 93.620 | 45.091 | 30.828 | 1.00 | 20.99 | D |
| ATOM | 3328 | CG2 | VAL | D | 43 | 94.456 | 42.827 | 31.539 | 1.00 | 19.79 | D |
| ATOM | 3329 | C | VAL | D | 43 | 90.968 | 43.744 | 30.164 | 1.00 | 20.50 | D |
| ATOM | 3330 | O | VAL | D | 43 | 91.045 | 43.513 | 28.959 | 1.00 | 19.49 | D |
| ATOM | 3331 | N | TRP | D | 44 | 89.987 | 44.466 | 30.690 | 1.00 | 21.49 | D |
| ATOM | 3332 | CA | TRP | D | 44 | 88.946 | 45.028 | 29.836 | 1.00 | 22.88 | D |
| ATOM | 3333 | CB | TRP | D | 44 | 87.685 | 45.326 | 30.649 | 1.00 | 21.57 | D |
| ATOM | 3334 | CG | TRP | D | 44 | 87.167 | 44.129 | 31.372 | 1.00 | 21.99 | D |
| ATOM | 3335 | CD2 | TRP | D | 44 | 86.280 | 43.125 | 30.854 | 1.00 | 22.20 | D |
| ATOM | 3336 | CE2 | TRP | D | 44 | 86.119 | 42.150 | 31.862 | 1.00 | 22.19 | D |
| ATOM | 3337 | CE3 | TRP | D | 44 | 85.611 | 42.951 | 29.634 | 1.00 | 20.96 | D |
| ATOM | 3338 | CD1 | TRP | D | 44 | 87.492 | 43.736 | 32.633 | 1.00 | 23.17 | D |
| ATOM | 3339 | NE1 | TRP | D | 44 | 86.868 | 42.548 | 32.937 | 1.00 | 23.70 | D |
| ATOM | 3340 | CZ2 | TRP | D | 44 | 85.311 | 41.016 | 31.693 | 1.00 | 24.30 | D |
| ATOM | 3341 | CZ3 | TRP | D | 44 | 84.807 | 41.824 | 29.461 | 1.00 | 22.81 | D |
| ATOM | 3342 | CH2 | TRP | D | 44 | 84.666 | 40.870 | 30.487 | 1.00 | 24.05 | D |
| ATOM | 3343 | C | TRP | D | 44 | 89.425 | 46.291 | 29.143 | 1.00 | 23.92 | D |
| ATOM | 3344 | O | TRP | D | 44 | 90.081 | 47.131 | 29.759 | 1.00 | 24.50 | D |
| ATOM | 3345 | N | CYS | D | 45 | 89.098 | 46.417 | 27.859 | 1.00 | 24.24 | D |
| ATOM | 3346 | CA | CYS | D | 45 | 89.498 | 47.580 | 27.069 | 1.00 | 26.23 | D |
| ATOM | 3347 | CB | CYS | D | 45 | 89.951 | 47.141 | 25.672 | 1.00 | 25.96 | D |
| ATOM | 3348 | SG | CYS | D | 45 | 91.422 | 46.098 | 25.665 | 1.00 | 25.42 | D |
| ATOM | 3349 | C | CYS | D | 45 | 88.377 | 48.608 | 26.950 | 1.00 | 27.07 | D |
| ATOM | 3350 | O | CYS | D | 45 | 88.612 | 49.749 | 26.549 | 1.00 | 28.23 | D |
| ATOM | 3351 | N | LEU | D | 46 | 87.157 | 48.193 | 27.273 | 1.00 | 27.18 | D |
| ATOM | 3352 | CA | LEU | D | 46 | 86.002 | 49.087 | 27.232 | 1.00 | 28.16 | D |
| ATOM | 3353 | CB | LEU | D | 46 | 84.907 | 48.525 | 26.320 | 1.00 | 27.82 | D |
| ATOM | 3354 | CG | LEU | D | 46 | 84.142 | 49.460 | 25.372 | 1.00 | 30.22 | D |
| ATOM | 3355 | CD1 | LEU | D | 46 | 82.792 | 48.827 | 25.040 | 1.00 | 29.72 | D |
| ATOM | 3356 | CD2 | LEU | D | 46 | 83.928 | 50.827 | 25.994 | 1.00 | 31.10 | D |
| ATOM | 3357 | C | LEU | D | 46 | 85.504 | 49.138 | 28.675 | 1.00 | 28.73 | D |
| ATOM | 3358 | O | LEU | D | 46 | 85.049 | 48.133 | 29.216 | 1.00 | 28.92 | D |
| ATOM | 3359 | N | PRO | D | 47 | 85.601 | 50.309 | 29.318 | 1.00 | 29.35 | D |
| ATOM | 3360 | CD | PRO | D | 47 | 86.116 | 51.554 | 28.717 | 1.00 | 28.33 | D |
| ATOM | 3361 | CA | PRO | D | 47 | 85.182 | 50.533 | 30.709 | 1.00 | 29.01 | D |
| ATOM | 3362 | CB | PRO | D | 47 | 85.139 | 52.051 | 30.806 | 1.00 | 29.32 | D |
| ATOM | 3363 | CG | PRO | D | 47 | 86.307 | 52.447 | 29.929 | 1.00 | 30.61 | D |
| ATOM | 3364 | C | PRO | D | 47 | 83.879 | 49.875 | 31.169 | 1.00 | 28.51 | D |
| ATOM | 3365 | O | PRO | D | 47 | 83.867 | 49.151 | 32.163 | 1.00 | 28.22 | D |
| ATOM | 3366 | N | VAL | D | 48 | 82.784 | 50.126 | 30.458 | 1.00 | 28.05 | D |
| ATOM | 3367 | CA | VAL | D | 48 | 81.492 | 49.545 | 30.826 | 1.00 | 27.41 | D |
| ATOM | 3368 | CB | VAL | D | 48 | 80.406 | 49.918 | 29.810 | 1.00 | 26.31 | D |
| ATOM | 3369 | CG1 | VAL | D | 48 | 79.955 | 51.345 | 30.027 | 1.00 | 30.25 | D |
| ATOM | 3370 | CG2 | VAL | D | 48 | 80.949 | 49.744 | 28.398 | 1.00 | 26.11 | D |
| ATOM | 3371 | C | VAL | D | 48 | 81.490 | 48.022 | 30.961 | 1.00 | 26.77 | D |
| ATOM | 3372 | O | VAL | D | 48 | 80.622 | 47.462 | 31.627 | 1.00 | 27.43 | D |
| ATOM | 3373 | N | LEU | D | 49 | 82.449 | 47.353 | 30.332 | 1.00 | 25.75 | D |
| ATOM | 3374 | CA | LEU | D | 49 | 82.517 | 45.898 | 30.395 | 1.00 | 27.21 | D |
| ATOM | 3375 | CB | LEU | D | 49 | 83.237 | 45.354 | 29.153 | 1.00 | 27.47 | D |
| ATOM | 3376 | CG | LEU | D | 49 | 82.405 | 44.886 | 27.944 | 1.00 | 29.74 | D |
| ATOM | 3377 | CD1 | LEU | D | 49 | 81.361 | 45.898 | 27.578 | 1.00 | 29.28 | D |
| ATOM | 3378 | CD2 | LEU | D | 49 | 83.329 | 44.627 | 26.753 | 1.00 | 29.72 | D |
| ATOM | 3379 | C | LEU | D | 49 | 83.185 | 45.374 | 31.674 | 1.00 | 27.86 | D |
| ATOM | 3380 | O | LEU | D | 49 | 83.246 | 44.163 | 31.900 | 1.00 | 25.45 | D |
| ATOM | 3381 | N | ARG | D | 50 | 83.680 | 46.283 | 32.508 | 1.00 | 29.82 | D |
| ATOM | 3382 | CA | ARG | D | 50 | 84.319 | 45.892 | 33.768 | 1.00 | 32.18 | D |
| ATOM | 3383 | CB | ARG | D | 50 | 84.900 | 47.105 | 34.509 | 1.00 | 35.49 | D |
| ATOM | 3384 | CG | ARG | D | 50 | 86.010 | 47.890 | 33.824 | 1.00 | 40.53 | D |
| ATOM | 3385 | CD | ARG | D | 50 | 86.524 | 48.968 | 34.786 | 1.00 | 42.89 | D |
| ATOM | 3386 | NE | ARG | D | 50 | 87.297 | 50.017 | 34.125 | 1.00 | 46.26 | D |
| ATOM | 3387 | CZ | ARG | D | 50 | 88.484 | 49.836 | 33.555 | 1.00 | 46.43 | D |
| ATOM | 3388 | NH1 | ARG | D | 50 | 89.049 | 48.636 | 33.564 | 1.00 | 46.42 | D |
| ATOM | 3389 | NH2 | ARG | D | 50 | 89.100 | 50.857 | 32.968 | 1.00 | 43.78 | D |
| ATOM | 3390 | C | ARG | D | 50 | 83.283 | 45.247 | 34.690 | 1.00 | 31.58 | D |
| ATOM | 3391 | O | ARG | D | 50 | 83.631 | 44.577 | 35.664 | 1.00 | 31.56 | D |
| ATOM | 3392 | N | GLN | D | 51 | 82.009 | 45.476 | 34.397 | 1.00 | 30.22 | D |
| ATOM | 3393 | CA | GLN | D | 51 | 80.942 | 44.921 | 35.221 | 1.00 | 30.10 | D |
| ATOM | 3394 | CB | GLN | D | 51 | 79.610 | 45.592 | 34.880 | 1.00 | 31.37 | D |
| ATOM | 3395 | CG | GLN | D | 51 | 79.194 | 45.469 | 33.426 | 1.00 | 33.44 | D |
| ATOM | 3396 | CD | GLN | D | 51 | 77.888 | 46.188 | 33.144 | 1.00 | 37.07 | D |
| ATOM | 3397 | OE1 | GLN | D | 51 | 76.835 | 45.824 | 33.678 | 1.00 | 36.72 | D |
| ATOM | 3398 | NE2 | GLN | D | 51 | 77.951 | 47.222 | 32.309 | 1.00 | 34.55 | D |
| ATOM | 3399 | C | GLN | D | 51 | 80.830 | 43.411 | 35.049 | 1.00 | 29.51 | D |

| ATOM | 3400 | O | GLN | D | 51 | 80.291 | 42.721 | 35.911 | 1.00 | 29.09 | D |
|------|------|------|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 3401 | N | PHE | D | 52 | 81.342 | 42.899 | 33.935 | 1.00 | 28.19 | D |
| ATOM | 3402 | CA | PHE | D | 52 | 81.300 | 41.468 | 33.676 | 1.00 | 26.27 | D |
| ATOM | 3403 | CB | PHE | D | 52 | 81.218 | 41.188 | 32.178 | 1.00 | 25.00 | D |
| ATOM | 3404 | CG | PHE | D | 52 | 80.030 | 41.801 | 31.513 | 1.00 | 23.07 | D |
| ATOM | 3405 | CD1 | PHE | D | 52 | 78.744 | 41.569 | 31.999 | 1.00 | 22.75 | D |
| ATOM | 3406 | CD2 | PHE | D | 52 | 80.188 | 42.594 | 30.380 | 1.00 | 23.46 | D |
| ATOM | 3407 | CE1 | PHE | D | 52 | 77.627 | 42.122 | 31.364 | 1.00 | 21.26 | D |
| ATOM | 3408 | CE2 | PHE | D | 52 | 79.079 | 43.151 | 29.735 | 1.00 | 21.92 | D |
| ATOM | 3409 | CZ | PHE | D | 52 | 77.799 | 42.913 | 30.231 | 1.00 | 21.69 | D |
| ATOM | 3410 | C | PHE | D | 52 | 82.547 | 40.797 | 34.217 | 1.00 | 27.11 | D |
| ATOM | 3411 | O | PHE | D | 52 | 83.477 | 41.461 | 34.669 | 1.00 | 27.64 | D |
| ATOM | 3412 | N | ARG | D | 53 | 82.556 | 39.471 | 34.152 | 1.00 | 27.25 | D |
| ATOM | 3413 | CA | ARG | D | 53 | 83.683 | 38.672 | 34.609 | 1.00 | 28.31 | D |
| ATOM | 3414 | CB | ARG | D | 53 | 83.347 | 37.976 | 35.939 | 1.00 | 32.75 | D |
| ATOM | 3415 | CG | ARG | D | 53 | 83.263 | 38.921 | 37.143 | 1.00 | 40.59 | D |
| ATOM | 3416 | CD | ARG | D | 53 | 82.418 | 38.325 | 38.269 | 1.00 | 45.99 | D |
| ATOM | 3417 | NE | ARG | D | 53 | 81.007 | 38.229 | 37.892 | 1.00 | 52.14 | D |
| ATOM | 3418 | CZ | ARG | D | 53 | 80.172 | 39.265 | 37.808 | 1.00 | 53.70 | D |
| ATOM | 3419 | NH1 | ARG | D | 53 | 80.597 | 40.493 | 38.080 | 1.00 | 53.85 | D |
| ATOM | 3420 | NH2 | ARG | D | 53 | 78.910 | 39.071 | 37.440 | 1.00 | 54.61 | D |
| ATOM | 3421 | C | ARG | D | 53 | 84.007 | 37.624 | 33.548 | 1.00 | 25.73 | D |
| ATOM | 3422 | O | ARG | D | 53 | 83.120 | 37.103 | 32.875 | 1.00 | 23.84 | D |
| ATOM | 3423 | N | PHE | D | 54 | 85.290 | 37.335 | 33.387 | 1.00 | 23.47 | D |
| ATOM | 3424 | CA | PHE | D | 54 | 85.716 | 36.336 | 32.425 | 1.00 | 19.92 | D |
| ATOM | 3425 | CB | PHE | D | 54 | 86.159 | 36.980 | 31.113 | 1.00 | 15.46 | D |
| ATOM | 3426 | CG | PHE | D | 54 | 86.346 | 35.994 | 30.007 | 1.00 | 17.29 | D |
| ATOM | 3427 | CD1 | PHE | D | 54 | 85.249 | 35.506 | 29.303 | 1.00 | 15.32 | D |
| ATOM | 3428 | CD2 | PHE | D | 54 | 87.615 | 35.503 | 29.701 | 1.00 | 15.07 | D |
| ATOM | 3429 | CE1 | PHE | D | 54 | 85.415 | 34.539 | 28.309 | 1.00 | 16.04 | D |
| ATOM | 3430 | CE2 | PHE | D | 54 | 87.788 | 34.535 | 28.709 | 1.00 | 13.99 | D |
| ATOM | 3431 | CZ | PHE | D | 54 | 86.688 | 34.055 | 28.014 | 1.00 | 14.35 | D |
| ATOM | 3432 | C | PHE | D | 54 | 86.879 | 35.598 | 33.055 | 1.00 | 18.63 | D |
| ATOM | 3433 | O | PHE | D | 54 | 87.922 | 36.188 | 33.329 | 1.00 | 19.50 | D |
| ATOM | 3434 | N | ASP | D | 55 | 86.676 | 34.312 | 33.309 | 1.00 | 19.05 | D |
| ATOM | 3435 | CA | ASP | D | 55 | 87.689 | 33.466 | 33.921 | 1.00 | 19.33 | D |
| ATOM | 3436 | CB | ASP | D | 55 | 87.084 | 32.100 | 34.237 | 1.00 | 21.38 | D |
| ATOM | 3437 | CG | ASP | D | 55 | 88.090 | 31.138 | 34.832 | 1.00 | 24.95 | D |
| ATOM | 3438 | OD1 | ASP | D | 55 | 89.264 | 31.528 | 35.021 | 1.00 | 27.01 | D |
| ATOM | 3439 | OD2 | ASP | D | 55 | 87.703 | 29.985 | 35.112 | 1.00 | 27.48 | D |
| ATOM | 3440 | C | ASP | D | 55 | 88.863 | 33.323 | 32.955 | 1.00 | 19.84 | D |
| ATOM | 3441 | O | ASP | D | 55 | 88.741 | 32.691 | 31.904 | 1.00 | 18.07 | D |
| ATOM | 3442 | N | PRO | D | 56 | 90.024 | 33.909 | 33.311 | 1.00 | 19.36 | D |
| ATOM | 3443 | CD | PRO | D | 56 | 90.285 | 34.584 | 34.593 | 1.00 | 16.09 | D |
| ATOM | 3444 | CA | PRO | D | 56 | 91.240 | 33.867 | 32.486 | 1.00 | 18.34 | D |
| ATOM | 3445 | CB | PRO | D | 56 | 92.228 | 34.729 | 33.278 | 1.00 | 19.78 | D |
| ATOM | 3446 | CG | PRO | D | 56 | 91.792 | 34.517 | 34.692 | 1.00 | 18.66 | D |
| ATOM | 3447 | C | PRO | D | 56 | 91.770 | 32.468 | 32.206 | 1.00 | 18.30 | D |
| ATOM | 3448 | O | PRO | D | 56 | 92.583 | 32.277 | 31.299 | 1.00 | 17.41 | D |
| ATOM | 3449 | N | GLN | D | 57 | 91.304 | 31.489 | 32.977 | 1.00 | 18.31 | D |
| ATOM | 3450 | CA | GLN | D | 57 | 91.744 | 30.114 | 32.781 | 1.00 | 18.39 | D |
| ATOM | 3451 | CB | GLN | D | 57 | 91.314 | 29.233 | 33.963 | 1.00 | 19.94 | D |
| ATOM | 3452 | CG | GLN | D | 57 | 91.738 | 27.773 | 33.856 | 1.00 | 18.50 | D |
| ATOM | 3453 | CD | GLN | D | 57 | 93.252 | 27.603 | 33.765 | 1.00 | 23.86 | D |
| ATOM | 3454 | OE1 | GLN | D | 57 | 94.000 | 28.110 | 34.612 | 1.00 | 23.68 | D |
| ATOM | 3455 | NE2 | GLN | D | 57 | 93.709 | 26.885 | 32.739 | 1.00 | 19.56 | D |
| ATOM | 3456 | C | GLN | D | 57 | 91.174 | 29.555 | 31.480 | 1.00 | 20.01 | D |
| ATOM | 3457 | O | GLN | D | 57 | 91.733 | 28.618 | 30.903 | 1.00 | 19.26 | D |
| ATOM | 3458 | N | PHE | D | 58 | 90.059 | 30.113 | 31.016 | 1.00 | 19.19 | D |
| ATOM | 3459 | CA | PHE | D | 58 | 89.490 | 29.629 | 29.765 | 1.00 | 20.37 | D |
| ATOM | 3460 | CB | PHE | D | 58 | 88.178 | 30.347 | 29.427 | 1.00 | 18.69 | D |
| ATOM | 3461 | CG | PHE | D | 58 | 87.587 | 29.912 | 28.114 | 1.00 | 20.67 | D |
| ATOM | 3462 | CD1 | PHE | D | 58 | 88.040 | 30.456 | 26.912 | 1.00 | 19.84 | D |
| ATOM | 3463 | CD2 | PHE | D | 58 | 86.640 | 28.891 | 28.070 | 1.00 | 19.87 | D |
| ATOM | 3464 | CE1 | PHE | D | 58 | 87.562 | 29.984 | 25.682 | 1.00 | 19.25 | D |
| ATOM | 3465 | CE2 | PHE | D | 58 | 86.156 | 28.411 | 26.844 | 1.00 | 20.67 | D |
| ATOM | 3466 | CZ | PHE | D | 58 | 86.623 | 28.961 | 25.652 | 1.00 | 19.50 | D |
| ATOM | 3467 | C | PHE | D | 58 | 90.508 | 29.892 | 28.659 | 1.00 | 20.46 | D |
| ATOM | 3468 | O | PHE | D | 58 | 90.745 | 29.049 | 27.790 | 1.00 | 20.36 | D |
| ATOM | 3469 | N | ALA | D | 59 | 91.115 | 31.070 | 28.716 | 1.00 | 20.85 | D |
| ATOM | 3470 | CA | ALA | D | 59 | 92.111 | 31.477 | 27.736 | 1.00 | 21.87 | D |
| ATOM | 3471 | CB | ALA | D | 59 | 92.458 | 32.959 | 27.937 | 1.00 | 20.20 | D |
| ATOM | 3472 | C | ALA | D | 59 | 93.374 | 30.618 | 27.819 | 1.00 | 22.41 | D |
| ATOM | 3473 | O | ALA | D | 59 | 93.877 | 30.151 | 26.796 | 1.00 | 22.54 | D |

| | | | | | | | | | | |
|------|------|-----|-----|---|----|---------|--------|--------|------|-------|---|
| ATOM | 3474 | N   | LEU | D | 60 | 93.890  | 30.409 | 29.030 | 1.00 | 21.24 | D |
| ATOM | 3475 | CA  | LEU | D | 60 | 95.101  | 29.601 | 29.188 | 1.00 | 22.31 | D |
| ATOM | 3476 | CB  | LEU | D | 60 | 95.501  | 29.474 | 30.663 | 1.00 | 22.79 | D |
| ATOM | 3477 | CG  | LEU | D | 60 | 96.063  | 30.698 | 31.393 | 1.00 | 25.87 | D |
| ATOM | 3478 | CD1 | LEU | D | 60 | 96.455  | 30.303 | 32.805 | 1.00 | 28.75 | D |
| ATOM | 3479 | CD2 | LEU | D | 60 | 97.270  | 31.223 | 30.670 | 1.00 | 28.42 | D |
| ATOM | 3480 | C   | LEU | D | 60 | 94.891  | 28.207 | 28.617 | 1.00 | 21.85 | D |
| ATOM | 3481 | O   | LEU | D | 60 | 95.731  | 27.691 | 27.875 | 1.00 | 22.48 | D |
| ATOM | 3482 | N   | THR | D | 61 | 93.763  | 27.600 | 28.966 | 1.00 | 19.32 | D |
| ATOM | 3483 | CA  | THR | D | 61 | 93.457  | 26.259 | 28.489 | 1.00 | 20.67 | D |
| ATOM | 3484 | CB  | THR | D | 61 | 92.175  | 25.721 | 29.158 | 1.00 | 20.04 | D |
| ATOM | 3485 | OG1 | THR | D | 61 | 92.419  | 25.539 | 30.558 | 1.00 | 23.09 | D |
| ATOM | 3486 | CG2 | THR | D | 61 | 91.759  | 24.393 | 28.546 | 1.00 | 21.15 | D |
| ATOM | 3487 | C   | THR | D | 61 | 93.283  | 26.240 | 26.974 | 1.00 | 19.50 | D |
| ATOM | 3488 | O   | THR | D | 61 | 93.805  | 25.363 | 26.288 | 1.00 | 18.76 | D |
| ATOM | 3489 | N   | ASN | D | 62 | 92.565  | 27.229 | 26.456 | 1.00 | 19.66 | D |
| ATOM | 3490 | CA  | ASN | D | 62 | 92.310  | 27.300 | 25.032 | 1.00 | 19.00 | D |
| ATOM | 3491 | CB  | ASN | D | 62 | 91.356  | 28.453 | 24.729 | 1.00 | 18.52 | D |
| ATOM | 3492 | CG  | ASN | D | 62 | 90.262  | 28.052 | 23.760 | 1.00 | 20.31 | D |
| ATOM | 3493 | OD1 | ASN | D | 62 | 89.726  | 26.942 | 23.833 | 1.00 | 19.27 | D |
| ATOM | 3494 | ND2 | ASN | D | 62 | 89.917  | 28.952 | 22.854 | 1.00 | 22.25 | D |
| ATOM | 3495 | C   | ASN | D | 62 | 93.599  | 27.445 | 24.244 | 1.00 | 19.63 | D |
| ATOM | 3496 | O   | ASN | D | 62 | 93.774  | 26.788 | 23.221 | 1.00 | 21.16 | D |
| ATOM | 3497 | N   | ILE | D | 63 | 94.509  | 28.290 | 24.724 | 1.00 | 19.68 | D |
| ATOM | 3498 | CA  | ILE | D | 63 | 95.779  | 28.481 | 24.033 | 1.00 | 18.76 | D |
| ATOM | 3499 | CB  | ILE | D | 63 | 96.587  | 29.660 | 24.645 | 1.00 | 18.72 | D |
| ATOM | 3500 | CG2 | ILE | D | 63 | 97.946  | 29.780 | 23.966 | 1.00 | 17.99 | D |
| ATOM | 3501 | CG1 | ILE | D | 63 | 95.813  | 30.968 | 24.471 | 1.00 | 17.09 | D |
| ATOM | 3502 | CD1 | ILE | D | 63 | 95.507  | 31.313 | 23.017 | 1.00 | 17.47 | D |
| ATOM | 3503 | C   | ILE | D | 63 | 96.613  | 27.195 | 24.094 | 1.00 | 18.86 | D |
| ATOM | 3504 | O   | ILE | D | 63 | 97.354  | 26.885 | 23.164 | 1.00 | 20.67 | D |
| ATOM | 3505 | N   | ALA | D | 64 | 96.497  | 26.448 | 25.188 | 1.00 | 18.22 | D |
| ATOM | 3506 | CA  | ALA | D | 64 | 97.244  | 25.193 | 25.316 | 1.00 | 20.33 | D |
| ATOM | 3507 | CB  | ALA | D | 64 | 97.039  | 24.574 | 26.708 | 1.00 | 17.30 | D |
| ATOM | 3508 | C   | ALA | D | 64 | 96.756  | 24.232 | 24.233 | 1.00 | 21.38 | D |
| ATOM | 3509 | O   | ALA | D | 64 | 97.536  | 23.459 | 23.677 | 1.00 | 23.44 | D |
| ATOM | 3510 | N   | VAL | D | 65 | 95.459  | 24.290 | 23.940 | 1.00 | 21.97 | D |
| ATOM | 3511 | CA  | VAL | D | 65 | 94.872  | 23.444 | 22.910 | 1.00 | 22.59 | D |
| ATOM | 3512 | CB  | VAL | D | 65 | 93.324  | 23.570 | 22.890 | 1.00 | 22.30 | D |
| ATOM | 3513 | CG1 | VAL | D | 65 | 92.744  | 22.781 | 21.728 | 1.00 | 17.73 | D |
| ATOM | 3514 | CG2 | VAL | D | 65 | 92.747  | 23.053 | 24.204 | 1.00 | 19.10 | D |
| ATOM | 3515 | C   | VAL | D | 65 | 95.441  | 23.832 | 21.541 | 1.00 | 23.65 | D |
| ATOM | 3516 | O   | VAL | D | 65 | 95.783  | 22.961 | 20.746 | 1.00 | 23.24 | D |
| ATOM | 3517 | N   | LEU | D | 66 | 95.552  | 25.133 | 21.271 | 1.00 | 25.03 | D |
| ATOM | 3518 | CA  | LEU | D | 66 | 96.102  | 25.580 | 19.991 | 1.00 | 26.10 | D |
| ATOM | 3519 | CB  | LEU | D | 66 | 96.104  | 27.111 | 19.870 | 1.00 | 23.98 | D |
| ATOM | 3520 | CG  | LEU | D | 66 | 94.826  | 27.953 | 19.969 | 1.00 | 25.20 | D |
| ATOM | 3521 | CD1 | LEU | D | 66 | 95.030  | 29.233 | 19.169 | 1.00 | 21.70 | D |
| ATOM | 3522 | CD2 | LEU | D | 66 | 93.629  | 27.211 | 19.435 | 1.00 | 26.16 | D |
| ATOM | 3523 | C   | LEU | D | 66 | 97.533  | 25.078 | 19.880 | 1.00 | 26.24 | D |
| ATOM | 3524 | O   | LEU | D | 66 | 97.971  | 24.667 | 18.816 | 1.00 | 27.10 | D |
| ATOM | 3525 | N   | LYS | D | 67 | 98.262  | 25.131 | 20.989 | 1.00 | 27.93 | D |
| ATOM | 3526 | CA  | LYS | D | 67 | 99.642  | 24.658 | 21.024 | 1.00 | 28.00 | D |
| ATOM | 3527 | CB  | LYS | D | 67 | 100.215 | 24.827 | 22.437 | 1.00 | 27.69 | D |
| ATOM | 3528 | CG  | LYS | D | 67 | 101.633 | 24.316 | 22.625 | 1.00 | 28.46 | D |
| ATOM | 3529 | CD  | LYS | D | 67 | 102.086 | 24.504 | 24.069 | 1.00 | 30.94 | D |
| ATOM | 3530 | CE  | LYS | D | 67 | 103.401 | 23.791 | 24.356 | 1.00 | 32.95 | D |
| ATOM | 3531 | NZ  | LYS | D | 67 | 104.517 | 24.279 | 23.503 | 1.00 | 35.64 | D |
| ATOM | 3532 | C   | LYS | D | 67 | 99.642  | 23.182 | 20.629 | 1.00 | 27.56 | D |
| ATOM | 3533 | O   | LYS | D | 67 | 100.414 | 22.759 | 19.767 | 1.00 | 27.65 | D |
| ATOM | 3534 | N   | HIS | D | 68 | 98.761  | 22.405 | 21.254 | 1.00 | 27.05 | D |
| ATOM | 3535 | CA  | HIS | D | 68 | 98.665  | 20.982 | 20.956 | 1.00 | 26.31 | D |
| ATOM | 3536 | CB  | HIS | D | 68 | 97.600  | 20.324 | 21.844 | 1.00 | 27.74 | D |
| ATOM | 3537 | CG  | HIS | D | 68 | 97.356  | 18.879 | 21.531 | 1.00 | 31.20 | D |
| ATOM | 3538 | CD2 | HIS | D | 68 | 97.801  | 17.748 | 22.130 | 1.00 | 31.26 | D |
| ATOM | 3539 | ND1 | HIS | D | 68 | 96.582  | 18.466 | 20.465 | 1.00 | 32.71 | D |
| ATOM | 3540 | CE1 | HIS | D | 68 | 96.560  | 17.146 | 20.423 | 1.00 | 31.32 | D |
| ATOM | 3541 | NE2 | HIS | D | 68 | 97.292  | 16.686 | 21.421 | 1.00 | 31.58 | D |
| ATOM | 3542 | C   | HIS | D | 68 | 98.341  | 20.757 | 19.483 | 1.00 | 25.27 | D |
| ATOM | 3543 | O   | HIS | D | 68 | 98.958  | 19.914 | 18.830 | 1.00 | 25.67 | D |
| ATOM | 3544 | N   | ASN | D | 69 | 97.386  | 21.521 | 18.959 | 1.00 | 22.00 | D |
| ATOM | 3545 | CA  | ASN | D | 69 | 96.986  | 21.398 | 17.561 | 1.00 | 23.20 | D |
| ATOM | 3546 | CB  | ASN | D | 69 | 95.706  | 22.210 | 17.307 | 1.00 | 23.27 | D |
| ATOM | 3547 | CG  | ASN | D | 69 | 94.447  | 21.504 | 17.805 | 1.00 | 24.20 | D |

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| ATOM | 3548 | OD1 | ASN | D | 69 | 94.521 | 20.536 | 18.562 | 1.00 | 26.69 | D |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 3549 | ND2 | ASN | D | 69 | 93.283 | 21.994 | 17.381 | 1.00 | 21.03 | D |
| ATOM | 3550 | C | ASN | D | 69 | 98.091 | 21.855 | 16.601 | 1.00 | 24.52 | D |
| ATOM | 3551 | O | ASN | D | 69 | 98.329 | 21.223 | 15.570 | 1.00 | 22.82 | D |
| ATOM | 3552 | N | LEU | D | 70 | 98.763 | 22.954 | 16.934 | 1.00 | 24.56 | D |
| ATOM | 3553 | CA | LEU | D | 70 | 99.831 | 23.459 | 16.078 | 1.00 | 26.89 | D |
| ATOM | 3554 | CB | LEU | D | 70 | 100.478 | 24.707 | 16.690 | 1.00 | 23.85 | D |
| ATOM | 3555 | CG | LEU | D | 70 | 101.619 | 25.306 | 15.857 | 1.00 | 22.71 | D |
| ATOM | 3556 | CD1 | LEU | D | 70 | 101.082 | 25.776 | 14.519 | 1.00 | 19.18 | D |
| ATOM | 3557 | CD2 | LEU | D | 70 | 102.254 | 26.472 | 16.592 | 1.00 | 23.62 | D |
| ATOM | 3558 | C | LEU | D | 70 | 100.900 | 22.388 | 15.882 | 1.00 | 28.63 | D |
| ATOM | 3559 | O | LEU | D | 70 | 101.413 | 22.210 | 14.780 | 1.00 | 27.56 | D |
| ATOM | 3560 | N | ASN | D | 71 | 101.224 | 21.687 | 16.967 | 1.00 | 31.13 | D |
| ATOM | 3561 | CA | ASN | D | 71 | 102.238 | 20.637 | 16.962 | 1.00 | 35.25 | D |
| ATOM | 3562 | CB | ASN | D | 71 | 102.393 | 20.052 | 18.370 | 1.00 | 35.30 | D |
| ATOM | 3563 | CG | ASN | D | 71 | 103.149 | 20.978 | 19.307 | 1.00 | 38.03 | D |
| ATOM | 3564 | OD1 | ASN | D | 71 | 103.197 | 20.751 | 20.518 | 1.00 | 40.05 | D |
| ATOM | 3565 | ND2 | ASN | D | 71 | 103.752 | 22.026 | 18.748 | 1.00 | 38.78 | D |
| ATOM | 3566 | C | ASN | D | 71 | 101.931 | 19.521 | 15.975 | 1.00 | 36.85 | D |
| ATOM | 3567 | O | ASN | D | 71 | 102.829 | 18.997 | 15.316 | 1.00 | 36.91 | D |
| ATOM | 3568 | N | SER | D | 72 | 100.660 | 19.157 | 15.876 | 1.00 | 38.08 | D |
| ATOM | 3569 | CA | SER | D | 72 | 100.261 | 18.104 | 14.961 | 1.00 | 39.44 | D |
| ATOM | 3570 | CB | SER | D | 72 | 98.847 | 17.623 | 15.306 | 1.00 | 40.69 | D |
| ATOM | 3571 | OG | SER | D | 72 | 98.529 | 16.427 | 14.611 | 1.00 | 44.84 | D |
| ATOM | 3572 | C | SER | D | 72 | 100.320 | 18.614 | 13.520 | 1.00 | 39.55 | D |
| ATOM | 3573 | O | SER | D | 72 | 100.798 | 17.915 | 12.625 | 1.00 | 38.61 | D |
| ATOM | 3574 | N | LEU | D | 73 | 99.846 | 19.839 | 13.305 | 1.00 | 40.64 | D |
| ATOM | 3575 | CA | LEU | D | 73 | 99.844 | 20.443 | 11.974 | 1.00 | 42.19 | D |
| ATOM | 3576 | CB | LEU | D | 73 | 99.085 | 21.768 | 11.990 | 1.00 | 42.17 | D |
| ATOM | 3577 | CG | LEU | D | 73 | 97.608 | 21.700 | 11.608 | 1.00 | 43.12 | D |
| ATOM | 3578 | CD1 | LEU | D | 73 | 96.891 | 20.664 | 12.443 | 1.00 | 44.19 | D |
| ATOM | 3579 | CD2 | LEU | D | 73 | 96.988 | 23.072 | 11.801 | 1.00 | 44.59 | D |
| ATOM | 3580 | C | LEU | D | 73 | 101.237 | 20.678 | 11.407 | 1.00 | 43.27 | D |
| ATOM | 3581 | O | LEU | D | 73 | 101.466 | 20.479 | 10.215 | 1.00 | 43.00 | D |
| ATOM | 3582 | N | ILE | D | 74 | 102.162 | 21.116 | 12.253 | 1.00 | 44.60 | D |
| ATOM | 3583 | CA | ILE | D | 74 | 103.529 | 21.364 | 11.812 | 1.00 | 46.44 | D |
| ATOM | 3584 | CB | ILE | D | 74 | 104.431 | 21.770 | 13.000 | 1.00 | 46.31 | D |
| ATOM | 3585 | CG2 | ILE | D | 74 | 105.893 | 21.792 | 12.571 | 1.00 | 46.14 | D |
| ATOM | 3586 | CG1 | ILE | D | 74 | 103.996 | 23.140 | 13.529 | 1.00 | 45.97 | D |
| ATOM | 3587 | CD1 | ILE | D | 74 | 104.683 | 23.561 | 14.812 | 1.00 | 43.97 | D |
| ATOM | 3588 | C | ILE | D | 74 | 104.077 | 20.095 | 11.166 | 1.00 | 48.14 | D |
| ATOM | 3589 | O | ILE | D | 74 | 104.724 | 20.147 | 10.119 | 1.00 | 48.28 | D |
| ATOM | 3590 | N | LYS | D | 75 | 103.800 | 18.957 | 11.795 | 1.00 | 49.68 | D |
| ATOM | 3591 | CA | LYS | D | 75 | 104.252 | 17.669 | 11.290 | 1.00 | 51.82 | D |
| ATOM | 3592 | CB | LYS | D | 75 | 104.060 | 16.589 | 12.356 | 1.00 | 52.85 | D |
| ATOM | 3593 | CG | LYS | D | 75 | 104.856 | 16.839 | 13.621 | 1.00 | 54.78 | D |
| ATOM | 3594 | CD | LYS | D | 75 | 104.517 | 15.831 | 14.704 | 1.00 | 57.28 | D |
| ATOM | 3595 | CE | LYS | D | 75 | 105.222 | 16.170 | 16.010 | 1.00 | 58.75 | D |
| ATOM | 3596 | NZ | LYS | D | 75 | 104.803 | 15.266 | 17.116 | 1.00 | 59.97 | D |
| ATOM | 3597 | C | LYS | D | 75 | 103.499 | 17.276 | 10.023 | 1.00 | 52.37 | D |
| ATOM | 3598 | O | LYS | D | 75 | 104.106 | 17.086 | 8.972 | 1.00 | 52.78 | D |
| ATOM | 3599 | N | ARG | D | 76 | 102.177 | 17.171 | 10.124 | 1.00 | 52.67 | D |
| ATOM | 3600 | CA | ARG | D | 76 | 101.353 | 16.783 | 8.986 | 1.00 | 52.67 | D |
| ATOM | 3601 | CB | ARG | D | 76 | 99.911 | 16.546 | 9.439 | 1.00 | 53.54 | D |
| ATOM | 3602 | CG | ARG | D | 76 | 99.764 | 15.339 | 10.346 | 1.00 | 55.62 | D |
| ATOM | 3603 | CD | ARG | D | 76 | 98.310 | 15.011 | 10.639 | 1.00 | 58.29 | D |
| ATOM | 3604 | NE | ARG | D | 76 | 97.628 | 16.107 | 11.319 | 1.00 | 61.07 | D |
| ATOM | 3605 | CZ | ARG | D | 76 | 96.437 | 16.000 | 11.900 | 1.00 | 62.21 | D |
| ATOM | 3606 | NH1 | ARG | D | 76 | 95.793 | 14.840 | 11.885 | 1.00 | 62.71 | D |
| ATOM | 3607 | NH2 | ARG | D | 76 | 95.889 | 17.055 | 12.492 | 1.00 | 61.94 | D |
| ATOM | 3608 | C | ARG | D | 76 | 101.375 | 17.761 | 7.816 | 1.00 | 52.35 | D |
| ATOM | 3609 | O | ARG | D | 76 | 100.691 | 17.550 | 6.817 | 1.00 | 52.65 | D |
| ATOM | 3610 | N | SER | D | 77 | 102.160 | 18.824 | 7.932 | 1.00 | 52.02 | D |
| ATOM | 3611 | CA | SER | D | 77 | 102.255 | 19.807 | 6.856 | 1.00 | 51.87 | D |
| ATOM | 3612 | CB | SER | D | 77 | 101.945 | 21.212 | 7.379 | 1.00 | 50.95 | D |
| ATOM | 3613 | OG | SER | D | 77 | 102.975 | 21.668 | 8.239 | 1.00 | 48.11 | D |
| ATOM | 3614 | C | SER | D | 77 | 103.667 | 19.789 | 6.287 | 1.00 | 52.25 | D |
| ATOM | 3615 | O | SER | D | 77 | 104.028 | 20.633 | 5.464 | 1.00 | 51.67 | D |
| ATOM | 3616 | N | ASN | D | 78 | 104.455 | 18.814 | 6.731 | 1.00 | 52.79 | D |
| ATOM | 3617 | CA | ASN | D | 78 | 105.841 | 18.675 | 6.301 | 1.00 | 53.67 | D |
| ATOM | 3618 | CB | ASN | D | 78 | 105.912 | 18.364 | 4.797 | 1.00 | 55.53 | D |
| ATOM | 3619 | CG | ASN | D | 78 | 107.298 | 17.901 | 4.355 | 1.00 | 57.31 | D |
| ATOM | 3620 | OD1 | ASN | D | 78 | 107.959 | 17.129 | 5.051 | 1.00 | 56.41 | D |
| ATOM | 3621 | ND2 | ASN | D | 78 | 107.732 | 18.360 | 3.184 | 1.00 | 58.05 | D |

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ATOM   3622  C   ASN D  78    106.549  19.985   6.632  1.00 52.90      D
ATOM   3623  O   ASN D  78    107.300  20.536   5.826  1.00 53.98      D
ATOM   3624  N   SER D  79    106.275  20.479   7.835  1.00 51.25      D
ATOM   3625  CA  SER D  79    106.856  21.715   8.341  1.00 49.59      D
ATOM   3626  CB  SER D  79    108.333  21.498   8.664  1.00 49.69      D
ATOM   3627  OG  SER D  79    108.472  20.604   9.753  1.00 52.23      D
ATOM   3628  C   SER D  79    106.711  22.931   7.437  1.00 47.21      D
ATOM   3629  O   SER D  79    107.699  23.588   7.111  1.00 47.49      D
ATOM   3630  N   THR D  80    105.483  23.235   7.032  1.00 44.68      D
ATOM   3631  CA  THR D  80    105.245  24.401   6.189  1.00 43.69      D
ATOM   3632  CB  THR D  80    103.928  24.274   5.407  1.00 45.12      D
ATOM   3633  OG1 THR D  80    103.976  23.112   4.570  1.00 47.94      D
ATOM   3634  CG2 THR D  80    103.706  25.505   4.541  1.00 44.11      D
ATOM   3635  C   THR D  80    105.166  25.634   7.094  1.00 42.94      D
ATOM   3636  O   THR D  80    104.225  25.783   7.874  1.00 41.60      D
ATOM   3637  N   ALA D  81    106.162  26.510   6.988  1.00 40.39      D
ATOM   3638  CA  ALA D  81    106.215  27.715   7.804  1.00 37.86      D
ATOM   3639  CB  ALA D  81    107.657  28.171   7.958  1.00 39.23      D
ATOM   3640  C   ALA D  81    105.372  28.846   7.234  1.00 36.29      D
ATOM   3641  O   ALA D  81    104.988  28.829   6.065  1.00 35.21      D
ATOM   3642  N   ALA D  82    105.087  29.829   8.079  1.00 34.40      D
ATOM   3643  CA  ALA D  82    104.294  30.984   7.685  1.00 32.51      D
ATOM   3644  CB  ALA D  82    103.915  31.789   8.920  1.00 32.45      D
ATOM   3645  C   ALA D  82    105.064  31.866   6.707  1.00 32.78      D
ATOM   3646  O   ALA D  82    106.294  31.913   6.740  1.00 30.87      D
ATOM   3647  N   THR D  83    104.333  32.561   5.839  1.00 32.79      D
ATOM   3648  CA  THR D  83    104.940  33.459   4.867  1.00 34.48      D
ATOM   3649  CB  THR D  83    104.195  33.429   3.521  1.00 35.64      D
ATOM   3650  OG1 THR D  83    104.179  32.094   3.006  1.00 38.88      D
ATOM   3651  CG2 THR D  83    104.880  34.342   2.521  1.00 35.33      D
ATOM   3652  C   THR D  83    104.886  34.887   5.401  1.00 35.30      D
ATOM   3653  O   THR D  83    103.827  35.355   5.824  1.00 36.88      D
ATOM   3654  N   ASN D  84    106.025  35.575   5.379  1.00 35.07      D
ATOM   3655  CA  ASN D  84    106.095  36.949   5.855  1.00 33.90      D
ATOM   3656  CB  ASN D  84    107.548  37.413   6.010  1.00 34.23      D
ATOM   3657  CG  ASN D  84    108.351  36.545   6.954  1.00 36.16      D
ATOM   3658  OD1 ASN D  84    107.895  36.195   8.043  1.00 34.99      D
ATOM   3659  ND2 ASN D  84    109.572  36.205   6.545  1.00 37.40      D
ATOM   3660  C   ASN D  84    105.419  37.879   4.865  1.00 34.74      D
ATOM   3661  O   ASN D  84    105.814  37.940   3.699  1.00 35.59      D
ATOM   3662  N   GLU D  85    104.401  38.599   5.327  1.00 34.09      D
ATOM   3663  CA  GLU D  85    103.695  39.561   4.489  1.00 32.99      D
ATOM   3664  CB  GLU D  85    102.239  39.714   4.939  1.00 35.56      D
ATOM   3665  CG  GLU D  85    101.370  38.475   4.746  1.00 40.80      D
ATOM   3666  CD  GLU D  85    101.019  38.215   3.291  1.00 43.32      D
ATOM   3667  OE1 GLU D  85    100.409  39.104   2.658  1.00 46.21      D
ATOM   3668  OE2 GLU D  85    101.345  37.119   2.782  1.00 44.58      D
ATOM   3669  C   GLU D  85    104.418  40.886   4.681  1.00 31.21      D
ATOM   3670  O   GLU D  85    105.220  41.024   5.602  1.00 32.36      D
ATOM   3671  N   VAL D  86    104.140  41.848   3.808  1.00 29.71      D
ATOM   3672  CA  VAL D  86    104.749  43.170   3.882  1.00 27.94      D
ATOM   3673  CB  VAL D  86    105.079  43.712   2.467  1.00 26.90      D
ATOM   3674  CG1 VAL D  86    105.569  45.166   2.543  1.00 23.11      D
ATOM   3675  CG2 VAL D  86    106.134  42.829   1.821  1.00 24.31      D
ATOM   3676  C   VAL D  86    103.767  44.114   4.574  1.00 29.81      D
ATOM   3677  O   VAL D  86    102.658  44.343   4.088  1.00 30.28      D
ATOM   3678  N   PRO D  87    104.162  44.666   5.729  1.00 29.08      D
ATOM   3679  CD  PRO D  87    105.356  44.310   6.509  1.00 29.37      D
ATOM   3680  CA  PRO D  87    103.306  45.583   6.485  1.00 30.85      D
ATOM   3681  CB  PRO D  87    104.083  45.791   7.786  1.00 30.80      D
ATOM   3682  CG  PRO D  87    104.878  44.551   7.920  1.00 30.83      D
ATOM   3683  C   PRO D  87    103.049  46.907   5.772  1.00 31.43      D
ATOM   3684  O   PRO D  87    103.863  47.357   4.968  1.00 31.78      D
ATOM   3685  N   GLU D  88    101.907  47.517   6.081  1.00 31.85      D
ATOM   3686  CA  GLU D  88    101.516  48.808   5.521  1.00 32.77      D
ATOM   3687  CB  GLU D  88    100.195  48.687   4.744  1.00 35.18      D
ATOM   3688  CG  GLU D  88     99.814  49.960   3.987  1.00 43.00      D
ATOM   3689  CD  GLU D  88     98.512  49.839   3.205  1.00 46.30      D
ATOM   3690  OE1 GLU D  88     97.439  49.745   3.837  1.00 47.40      D
ATOM   3691  OE2 GLU D  88     98.564  49.840   1.954  1.00 48.25      D
ATOM   3692  C   GLU D  88    101.338  49.748   6.721  1.00 31.26      D
ATOM   3693  O   GLU D  88    100.556  49.457   7.630  1.00 31.21      D
ATOM   3694  N   VAL D  89    102.060  50.864   6.728  1.00 28.43      D
ATOM   3695  CA  VAL D  89    101.988  51.806   7.842  1.00 26.87      D
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| ATOM | 3696 | CB | VAL | D | 89 | 103.385 | 52.024 | 8.454 | 1.00 | 26.58 | D |
|------|------|-----|-----|---|----|---------|--------|--------|------|-------|---|
| ATOM | 3697 | CG1 | VAL | D | 89 | 103.277 | 52.886 | 9.699 | 1.00 | 26.80 | D |
| ATOM | 3698 | CG2 | VAL | D | 89 | 104.021 | 50.679 | 8.787 | 1.00 | 24.58 | D |
| ATOM | 3699 | C | VAL | D | 89 | 101.389 | 53.174 | 7.505 | 1.00 | 27.02 | D |
| ATOM | 3700 | O | VAL | D | 89 | 101.698 | 53.772 | 6.473 | 1.00 | 26.22 | D |
| ATOM | 3701 | N | THR | D | 90 | 100.530 | 53.662 | 8.394 | 1.00 | 26.33 | D |
| ATOM | 3702 | CA | THR | D | 90 | 99.881 | 54.955 | 8.219 | 1.00 | 26.05 | D |
| ATOM | 3703 | CB | THR | D | 90 | 98.414 | 54.802 | 7.769 | 1.00 | 27.24 | D |
| ATOM | 3704 | OG1 | THR | D | 90 | 98.359 | 54.063 | 6.543 | 1.00 | 31.41 | D |
| ATOM | 3705 | CG2 | THR | D | 90 | 97.786 | 56.163 | 7.545 | 1.00 | 28.57 | D |
| ATOM | 3706 | C | THR | D | 90 | 99.883 | 55.698 | 9.546 | 1.00 | 24.83 | D |
| ATOM | 3707 | O | THR | D | 90 | 99.542 | 55.120 | 10.581 | 1.00 | 25.45 | D |
| ATOM | 3708 | N | VAL | D | 91 | 100.266 | 56.972 | 9.512 | 1.00 | 22.04 | D |
| ATOM | 3709 | CA | VAL | D | 91 | 100.300 | 57.791 | 10.716 | 1.00 | 21.50 | D |
| ATOM | 3710 | CB | VAL | D | 91 | 101.749 | 58.280 | 11.031 | 1.00 | 23.04 | D |
| ATOM | 3711 | CG1 | VAL | D | 91 | 101.737 | 59.245 | 12.225 | 1.00 | 22.74 | D |
| ATOM | 3712 | CG2 | VAL | D | 91 | 102.650 | 57.082 | 11.340 | 1.00 | 20.38 | D |
| ATOM | 3713 | C | VAL | D | 91 | 99.369 | 58.993 | 10.553 | 1.00 | 21.65 | D |
| ATOM | 3714 | O | VAL | D | 91 | 99.357 | 59.653 | 9.509 | 1.00 | 21.70 | D |
| ATOM | 3715 | N | PHE | D | 92 | 98.573 | 59.252 | 11.586 | 1.00 | 21.34 | D |
| ATOM | 3716 | CA | PHE | D | 92 | 97.633 | 60.363 | 11.580 | 1.00 | 21.48 | D |
| ATOM | 3717 | CB | PHE | D | 92 | 96.370 | 59.985 | 10.788 | 1.00 | 21.60 | D |
| ATOM | 3718 | CG | PHE | D | 92 | 95.652 | 58.771 | 11.314 | 1.00 | 22.22 | D |
| ATOM | 3719 | CD1 | PHE | D | 92 | 94.601 | 58.902 | 12.215 | 1.00 | 24.10 | D |
| ATOM | 3720 | CD2 | PHE | D | 92 | 96.038 | 57.495 | 10.925 | 1.00 | 24.53 | D |
| ATOM | 3721 | CE1 | PHE | D | 92 | 93.940 | 57.774 | 12.724 | 1.00 | 22.72 | D |
| ATOM | 3722 | CE2 | PHE | D | 92 | 95.386 | 56.355 | 11.428 | 1.00 | 23.87 | D |
| ATOM | 3723 | CZ | PHE | D | 92 | 94.335 | 56.501 | 12.329 | 1.00 | 21.18 | D |
| ATOM | 3724 | C | PHE | D | 92 | 97.303 | 60.700 | 13.030 | 1.00 | 22.72 | D |
| ATOM | 3725 | O | PHE | D | 92 | 97.607 | 59.921 | 13.933 | 1.00 | 22.31 | D |
| ATOM | 3726 | N | SER | D | 93 | 96.696 | 61.859 | 13.261 | 1.00 | 22.45 | D |
| ATOM | 3727 | CA | SER | D | 93 | 96.366 | 62.262 | 14.623 | 1.00 | 21.69 | D |
| ATOM | 3728 | CB | SER | D | 93 | 96.599 | 63.764 | 14.799 | 1.00 | 20.96 | D |
| ATOM | 3729 | OG | SER | D | 93 | 95.696 | 64.508 | 14.010 | 1.00 | 25.08 | D |
| ATOM | 3730 | C | SER | D | 93 | 94.931 | 61.913 | 14.990 | 1.00 | 21.02 | D |
| ATOM | 3731 | O | SER | D | 93 | 94.078 | 61.755 | 14.127 | 1.00 | 20.62 | D |
| ATOM | 3732 | N | LYS | D | 94 | 94.676 | 61.791 | 16.283 | 1.00 | 20.66 | D |
| ATOM | 3733 | CA | LYS | D | 94 | 93.350 | 61.453 | 16.768 | 1.00 | 24.11 | D |
| ATOM | 3734 | CB | LYS | D | 94 | 93.444 | 60.985 | 18.223 | 1.00 | 24.91 | D |
| ATOM | 3735 | CG | LYS | D | 94 | 92.121 | 60.605 | 18.865 | 1.00 | 29.49 | D |
| ATOM | 3736 | CD | LYS | D | 94 | 92.353 | 60.101 | 20.293 | 1.00 | 32.97 | D |
| ATOM | 3737 | CE | LYS | D | 94 | 91.050 | 59.909 | 21.052 | 1.00 | 33.37 | D |
| ATOM | 3738 | NZ | LYS | D | 94 | 90.175 | 58.897 | 20.399 | 1.00 | 34.08 | D |
| ATOM | 3739 | C | LYS | D | 94 | 92.406 | 62.646 | 16.654 | 1.00 | 24.40 | D |
| ATOM | 3740 | O | LYS | D | 94 | 91.224 | 62.495 | 16.356 | 1.00 | 24.55 | D |
| ATOM | 3741 | N | SER | D | 95 | 92.935 | 63.834 | 16.894 | 1.00 | 25.54 | D |
| ATOM | 3742 | CA | SER | D | 95 | 92.133 | 65.040 | 16.815 | 1.00 | 29.22 | D |
| ATOM | 3743 | CB | SER | D | 95 | 91.932 | 65.643 | 18.208 | 1.00 | 30.47 | D |
| ATOM | 3744 | OG | SER | D | 95 | 91.236 | 64.746 | 19.060 | 1.00 | 36.11 | D |
| ATOM | 3745 | C | SER | D | 95 | 92.843 | 66.046 | 15.932 | 1.00 | 29.71 | D |
| ATOM | 3746 | O | SER | D | 95 | 93.993 | 65.834 | 15.531 | 1.00 | 29.68 | D |
| ATOM | 3747 | N | PRO | D | 96 | 92.159 | 67.146 | 15.588 | 1.00 | 29.93 | D |
| ATOM | 3748 | CD | PRO | D | 96 | 90.760 | 67.532 | 15.843 | 1.00 | 31.14 | D |
| ATOM | 3749 | CA | PRO | D | 96 | 92.836 | 68.129 | 14.747 | 1.00 | 29.29 | D |
| ATOM | 3750 | CB | PRO | D | 96 | 91.714 | 69.097 | 14.369 | 1.00 | 31.65 | D |
| ATOM | 3751 | CG | PRO | D | 96 | 90.777 | 69.010 | 15.545 | 1.00 | 30.66 | D |
| ATOM | 3752 | C | PRO | D | 96 | 93.939 | 68.765 | 15.587 | 1.00 | 27.35 | D |
| ATOM | 3753 | O | PRO | D | 96 | 93.818 | 68.904 | 16.806 | 1.00 | 24.86 | D |
| ATOM | 3754 | N | VAL | D | 97 | 95.025 | 69.127 | 14.929 | 1.00 | 26.81 | D |
| ATOM | 3755 | CA | VAL | D | 97 | 96.158 | 69.706 | 15.615 | 1.00 | 29.25 | D |
| ATOM | 3756 | CB | VAL | D | 97 | 97.438 | 69.501 | 14.783 | 1.00 | 31.49 | D |
| ATOM | 3757 | CG1 | VAL | D | 97 | 98.652 | 69.998 | 15.556 | 1.00 | 33.50 | D |
| ATOM | 3758 | CG2 | VAL | D | 97 | 97.583 | 68.029 | 14.415 | 1.00 | 34.03 | D |
| ATOM | 3759 | C | VAL | D | 97 | 96.007 | 71.196 | 15.910 | 1.00 | 28.80 | D |
| ATOM | 3760 | O | VAL | D | 97 | 95.749 | 71.998 | 15.012 | 1.00 | 28.78 | D |
| ATOM | 3761 | N | THR | D | 98 | 96.144 | 71.559 | 17.178 | 1.00 | 27.47 | D |
| ATOM | 3762 | CA | THR | D | 98 | 96.091 | 72.960 | 17.572 | 1.00 | 26.55 | D |
| ATOM | 3763 | CB | THR | D | 98 | 94.723 | 73.365 | 18.209 | 1.00 | 26.16 | D |
| ATOM | 3764 | OG1 | THR | D | 98 | 94.684 | 72.961 | 19.575 | 1.00 | 31.83 | D |
| ATOM | 3765 | CG2 | THR | D | 98 | 93.567 | 72.717 | 17.469 | 1.00 | 23.66 | D |
| ATOM | 3766 | C | THR | D | 98 | 97.220 | 73.114 | 18.581 | 1.00 | 25.73 | D |
| ATOM | 3767 | O | THR | D | 98 | 97.260 | 72.412 | 19.591 | 1.00 | 27.12 | D |
| ATOM | 3768 | N | LEU | D | 99 | 98.159 | 74.005 | 18.285 | 1.00 | 26.12 | D |
| ATOM | 3769 | CA | LEU | D | 99 | 99.307 | 74.236 | 19.156 | 1.00 | 27.47 | D |

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| ATOM | 3770 | CB | LEU | D | 99 | 100.089 | 75.459 | 18.675 | 1.00 | 31.04 | D |
|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| ATOM | 3771 | CG | LEU | D | 99 | 100.758 | 75.309 | 17.310 | 1.00 | 33.09 | D |
| ATOM | 3772 | CD1 | LEU | D | 99 | 101.458 | 76.607 | 16.940 | 1.00 | 36.20 | D |
| ATOM | 3773 | CD2 | LEU | D | 99 | 101.754 | 74.165 | 17.361 | 1.00 | 35.56 | D |
| ATOM | 3774 | C | LEU | D | 99 | 98.935 | 74.416 | 20.621 | 1.00 | 26.08 | D |
| ATOM | 3775 | O | LEU | D | 99 | 98.077 | 75.222 | 20.946 | 1.00 | 25.97 | D |
| ATOM | 3776 | N | GLY | D | 100 | 99.585 | 73.654 | 21.500 | 1.00 | 26.97 | D |
| ATOM | 3777 | CA | GLY | D | 100 | 99.310 | 73.749 | 22.924 | 1.00 | 26.03 | D |
| ATOM | 3778 | C | GLY | D | 100 | 98.233 | 72.798 | 23.422 | 1.00 | 26.02 | D |
| ATOM | 3779 | O | GLY | D | 100 | 98.020 | 72.662 | 24.629 | 1.00 | 25.51 | D |
| ATOM | 3780 | N | GLN | D | 101 | 97.553 | 72.143 | 22.491 | 1.00 | 25.73 | D |
| ATOM | 3781 | CA | GLN | D | 101 | 96.490 | 71.199 | 22.820 | 1.00 | 28.13 | D |
| ATOM | 3782 | CB | GLN | D | 101 | 95.372 | 71.297 | 21.776 | 1.00 | 32.24 | D |
| ATOM | 3783 | CG | GLN | D | 101 | 94.617 | 69.981 | 21.560 | 1.00 | 38.65 | D |
| ATOM | 3784 | CD | GLN | D | 101 | 94.680 | 69.459 | 20.115 | 1.00 | 41.08 | D |
| ATOM | 3785 | OE1 | GLN | D | 101 | 95.760 | 69.348 | 19.511 | 1.00 | 38.18 | D |
| ATOM | 3786 | NE2 | GLN | D | 101 | 93.515 | 69.119 | 19.566 | 1.00 | 40.87 | D |
| ATOM | 3787 | C | GLN | D | 101 | 96.994 | 69.756 | 22.861 | 1.00 | 25.22 | D |
| ATOM | 3788 | O | GLN | D | 101 | 97.477 | 69.245 | 21.857 | 1.00 | 24.55 | D |
| ATOM | 3789 | N | PRO | D | 102 | 96.885 | 69.078 | 24.019 | 1.00 | 24.18 | D |
| ATOM | 3790 | CD | PRO | D | 102 | 96.436 | 69.544 | 25.343 | 1.00 | 22.22 | D |
| ATOM | 3791 | CA | PRO | D | 102 | 97.359 | 67.683 | 24.080 | 1.00 | 22.76 | D |
| ATOM | 3792 | CB | PRO | D | 102 | 96.983 | 67.253 | 25.494 | 1.00 | 22.02 | D |
| ATOM | 3793 | CG | PRO | D | 102 | 97.088 | 68.542 | 26.274 | 1.00 | 22.44 | D |
| ATOM | 3794 | C | PRO | D | 102 | 96.649 | 66.845 | 23.015 | 1.00 | 21.72 | D |
| ATOM | 3795 | O | PRO | D | 102 | 95.429 | 66.922 | 22.876 | 1.00 | 22.65 | D |
| ATOM | 3796 | N | ASN | D | 103 | 97.409 | 66.055 | 22.264 | 1.00 | 19.84 | D |
| ATOM | 3797 | CA | ASN | D | 103 | 96.833 | 65.225 | 21.209 | 1.00 | 17.89 | D |
| ATOM | 3798 | CB | ASN | D | 103 | 97.112 | 65.856 | 19.838 | 1.00 | 16.30 | D |
| ATOM | 3799 | CG | ASN | D | 103 | 96.005 | 65.587 | 18.824 | 1.00 | 16.50 | D |
| ATOM | 3800 | OD1 | ASN | D | 103 | 95.552 | 64.446 | 18.636 | 1.00 | 16.80 | D |
| ATOM | 3801 | ND2 | ASN | D | 103 | 95.569 | 66.643 | 18.160 | 1.00 | 14.61 | D |
| ATOM | 3802 | C | ASN | D | 103 | 97.410 | 63.805 | 21.248 | 1.00 | 17.24 | D |
| ATOM | 3803 | O | ASN | D | 103 | 98.199 | 63.473 | 22.129 | 1.00 | 15.74 | D |
| ATOM | 3804 | N | ILE | D | 104 | 97.010 | 62.977 | 20.284 | 1.00 | 17.39 | D |
| ATOM | 3805 | CA | ILE | D | 104 | 97.465 | 61.595 | 20.198 | 1.00 | 15.30 | D |
| ATOM | 3806 | CB | ILE | D | 104 | 96.402 | 60.627 | 20.755 | 1.00 | 17.89 | D |
| ATOM | 3807 | CG2 | ILE | D | 104 | 96.818 | 59.175 | 20.498 | 1.00 | 13.27 | D |
| ATOM | 3808 | CG1 | ILE | D | 104 | 96.202 | 60.886 | 22.253 | 1.00 | 18.46 | D |
| ATOM | 3809 | CD1 | ILE | D | 104 | 95.179 | 59.965 | 22.895 | 1.00 | 17.98 | D |
| ATOM | 3810 | C | ILE | D | 104 | 97.760 | 61.185 | 18.763 | 1.00 | 17.15 | D |
| ATOM | 3811 | O | ILE | D | 104 | 96.887 | 61.283 | 17.902 | 1.00 | 18.07 | D |
| ATOM | 3812 | N | LEU | D | 105 | 98.987 | 60.727 | 18.509 | 1.00 | 16.66 | D |
| ATOM | 3813 | CA | LEU | D | 105 | 99.370 | 60.272 | 17.177 | 1.00 | 16.59 | D |
| ATOM | 3814 | CB | LEU | D | 105 | 100.864 | 60.482 | 16.895 | 1.00 | 17.56 | D |
| ATOM | 3815 | CG | LEU | D | 105 | 101.375 | 61.926 | 16.842 | 1.00 | 21.66 | D |
| ATOM | 3816 | CD1 | LEU | D | 105 | 102.811 | 61.943 | 16.302 | 1.00 | 21.26 | D |
| ATOM | 3817 | CD2 | LEU | D | 105 | 100.460 | 62.771 | 15.951 | 1.00 | 21.56 | D |
| ATOM | 3818 | C | LEU | D | 105 | 99.061 | 58.804 | 17.128 | 1.00 | 17.13 | D |
| ATOM | 3819 | O | LEU | D | 105 | 99.368 | 58.056 | 18.056 | 1.00 | 18.35 | D |
| ATOM | 3820 | N | ILE | D | 106 | 98.432 | 58.399 | 16.039 | 1.00 | 17.88 | D |
| ATOM | 3821 | CA | ILE | D | 106 | 98.045 | 57.016 | 15.839 | 1.00 | 17.14 | D |
| ATOM | 3822 | CB | ILE | D | 106 | 96.525 | 56.939 | 15.492 | 1.00 | 16.99 | D |
| ATOM | 3823 | CG2 | ILE | D | 106 | 96.093 | 55.496 | 15.318 | 1.00 | 15.63 | D |
| ATOM | 3824 | CG1 | ILE | D | 106 | 95.711 | 57.619 | 16.604 | 1.00 | 19.04 | D |
| ATOM | 3825 | CD1 | ILE | D | 106 | 94.238 | 57.877 | 16.260 | 1.00 | 16.48 | D |
| ATOM | 3826 | C | ILE | D | 106 | 98.876 | 56.431 | 14.700 | 1.00 | 17.19 | D |
| ATOM | 3827 | O | ILE | D | 106 | 98.941 | 57.004 | 13.618 | 1.00 | 16.06 | D |
| ATOM | 3828 | N | CYS | D | 107 | 99.540 | 55.312 | 14.966 | 1.00 | 18.84 | D |
| ATOM | 3829 | CA | CYS | D | 107 | 100.339 | 54.637 | 13.954 | 1.00 | 19.74 | D |
| ATOM | 3830 | C | CYS | D | 107 | 99.634 | 53.323 | 13.670 | 1.00 | 20.17 | D |
| ATOM | 3831 | O | CYS | D | 107 | 99.632 | 52.421 | 14.507 | 1.00 | 20.08 | D |
| ATOM | 3832 | CB | CYS | D | 107 | 101.755 | 54.349 | 14.453 | 1.00 | 22.00 | D |
| ATOM | 3833 | SG | CYS | D | 107 | 102.800 | 53.514 | 13.211 | 1.00 | 28.61 | D |
| ATOM | 3834 | N | LEU | D | 108 | 99.027 | 53.221 | 12.493 | 1.00 | 19.48 | D |
| ATOM | 3835 | CA | LEU | D | 108 | 98.313 | 52.015 | 12.113 | 1.00 | 19.67 | D |
| ATOM | 3836 | CB | LEU | D | 108 | 97.024 | 52.391 | 11.369 | 1.00 | 19.98 | D |
| ATOM | 3837 | CG | LEU | D | 108 | 95.977 | 51.358 | 10.925 | 1.00 | 20.40 | D |
| ATOM | 3838 | CD1 | LEU | D | 108 | 95.883 | 51.366 | 9.412 | 1.00 | 20.15 | D |
| ATOM | 3839 | CD2 | LEU | D | 108 | 96.301 | 49.971 | 11.454 | 1.00 | 19.44 | D |
| ATOM | 3840 | C | LEU | D | 108 | 99.207 | 51.145 | 11.237 | 1.00 | 19.84 | D |
| ATOM | 3841 | O | LEU | D | 108 | 99.657 | 51.563 | 10.170 | 1.00 | 20.11 | D |
| ATOM | 3842 | N | VAL | D | 109 | 99.473 | 49.940 | 11.721 | 1.00 | 19.32 | D |
| ATOM | 3843 | CA | VAL | D | 109 | 100.289 | 48.972 | 11.016 | 1.00 | 19.64 | D |

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ATOM    3844  CB   VAL D 109      101.368  48.402  11.958  1.00 19.40       D
ATOM    3845  CG1  VAL D 109      102.290  47.474  11.202  1.00 18.01       D
ATOM    3846  CG2  VAL D 109      102.155  49.560  12.590  1.00 17.30       D
ATOM    3847  C    VAL D 109       99.321  47.876  10.568  1.00 21.45       D
ATOM    3848  O    VAL D 109       98.845  47.079  11.382  1.00 22.65       D
ATOM    3849  N    ASP D 110       99.022  47.861   9.274  1.00 22.00       D
ATOM    3850  CA   ASP D 110       98.086  46.901   8.689  1.00 23.80       D
ATOM    3851  CB   ASP D 110       97.156  47.648   7.728  1.00 24.68       D
ATOM    3852  CG   ASP D 110       95.790  47.002   7.603  1.00 26.64       D
ATOM    3853  OD1  ASP D 110       95.582  45.915   8.177  1.00 28.80       D
ATOM    3854  OD2  ASP D 110       94.920  47.591   6.926  1.00 27.99       D
ATOM    3855  C    ASP D 110       98.802  45.756   7.944  1.00 23.77       D
ATOM    3856  O    ASP D 110      100.005  45.831   7.684  1.00 22.82       D
ATOM    3857  N    ASN D 111       98.044  44.711   7.604  1.00 23.55       D
ATOM    3858  CA   ASN D 111       98.548  43.530   6.889  1.00 23.79       D
ATOM    3859  CB   ASN D 111       98.880  43.867   5.425  1.00 25.36       D
ATOM    3860  CG   ASN D 111       99.079  42.610   4.562  1.00 29.95       D
ATOM    3861  OD1  ASN D 111       99.981  42.547   3.724  1.00 29.58       D
ATOM    3862  ND2  ASN D 111       98.220  41.611   4.761  1.00 30.51       D
ATOM    3863  C    ASN D 111       99.786  42.941   7.556  1.00 22.70       D
ATOM    3864  O    ASN D 111      100.834  42.784   6.929  1.00 22.97       D
ATOM    3865  N    ILE D 112       99.656  42.612   8.835  1.00 22.14       D
ATOM    3866  CA   ILE D 112      100.754  42.038   9.598  1.00 20.20       D
ATOM    3867  CB   ILE D 112      100.746  42.536  11.055  1.00 18.82       D
ATOM    3868  CG2  ILE D 112      101.926  41.950  11.808  1.00 15.77       D
ATOM    3869  CG1  ILE D 112      100.770  44.058  11.103  1.00 19.09       D
ATOM    3870  CD1  ILE D 112      100.630  44.602  12.514  1.00 21.18       D
ATOM    3871  C    ILE D 112      100.666  40.512   9.659  1.00 21.41       D
ATOM    3872  O    ILE D 112       99.626  39.960  10.002  1.00 22.04       D
ATOM    3873  N    PHE D 113      101.765  39.838   9.338  1.00 21.35       D
ATOM    3874  CA   PHE D 113      101.818  38.386   9.409  1.00 19.93       D
ATOM    3875  CB   PHE D 113      100.822  37.726   8.462  1.00 21.28       D
ATOM    3876  CG   PHE D 113      100.537  36.306   8.825  1.00 20.91       D
ATOM    3877  CD1  PHE D 113       99.630  36.012   9.838  1.00 19.85       D
ATOM    3878  CD2  PHE D 113      101.244  35.261   8.230  1.00 22.61       D
ATOM    3879  CE1  PHE D 113       99.430  34.698  10.264  1.00 20.63       D
ATOM    3880  CE2  PHE D 113      101.054  33.942   8.646  1.00 21.21       D
ATOM    3881  CZ   PHE D 113      100.144  33.660   9.669  1.00 20.87       D
ATOM    3882  C    PHE D 113      103.201  37.871   9.071  1.00 19.98       D
ATOM    3883  O    PHE D 113      103.762  38.238   8.044  1.00 20.80       D
ATOM    3884  N    PRO D 114      103.765  37.005   9.925  1.00 21.26       D
ATOM    3885  CD   PRO D 114      105.101  36.414   9.732  1.00 21.94       D
ATOM    3886  CA   PRO D 114      103.150  36.518  11.166  1.00 21.41       D
ATOM    3887  CB   PRO D 114      104.117  35.424  11.625  1.00 21.03       D
ATOM    3888  CG   PRO D 114      105.441  35.912  11.115  1.00 22.98       D
ATOM    3889  C    PRO D 114      103.002  37.648  12.185  1.00 21.84       D
ATOM    3890  O    PRO D 114      103.621  38.711  12.034  1.00 20.41       D
ATOM    3891  N    PRO D 115      102.167  37.441  13.222  1.00 22.52       D
ATOM    3892  CD   PRO D 115      101.314  36.256  13.445  1.00 22.08       D
ATOM    3893  CA   PRO D 115      101.937  38.448  14.266  1.00 21.19       D
ATOM    3894  CB   PRO D 115      100.730  37.895  15.025  1.00 20.92       D
ATOM    3895  CG   PRO D 115      100.917  36.410  14.902  1.00 19.88       D
ATOM    3896  C    PRO D 115      103.139  38.683  15.171  1.00 21.62       D
ATOM    3897  O    PRO D 115      103.127  38.336  16.356  1.00 22.92       D
ATOM    3898  N    VAL D 116      104.179  39.263  14.588  1.00 21.58       D
ATOM    3899  CA   VAL D 116      105.405  39.598  15.300  1.00 22.53       D
ATOM    3900  CB   VAL D 116      106.520  38.554  15.067  1.00 24.90       D
ATOM    3901  CG1  VAL D 116      107.817  39.035  15.713  1.00 24.06       D
ATOM    3902  CG2  VAL D 116      106.104  37.195  15.641  1.00 24.88       D
ATOM    3903  C    VAL D 116      105.855  40.929  14.708  1.00 21.86       D
ATOM    3904  O    VAL D 116      106.114  41.027  13.509  1.00 20.87       D
ATOM    3905  N    VAL D 117      105.935  41.962  15.534  1.00 20.65       D
ATOM    3906  CA   VAL D 117      106.338  43.255  15.007  1.00 21.60       D
ATOM    3907  CB   VAL D 117      105.126  43.978  14.345  1.00 18.11       D
ATOM    3908  CG1  VAL D 117      104.156  44.473  15.403  1.00 16.63       D
ATOM    3909  CG2  VAL D 117      105.599  45.101  13.469  1.00 17.02       D
ATOM    3910  C    VAL D 117      106.928  44.137  16.092  1.00 23.84       D
ATOM    3911  O    VAL D 117      106.677  43.936  17.280  1.00 24.78       D
ATOM    3912  N    ASN D 118      107.719  45.113  15.670  1.00 27.93       D
ATOM    3913  CA   ASN D 118      108.348  46.051  16.593  1.00 30.45       D
ATOM    3914  CB   ASN D 118      109.866  45.898  16.538  1.00 33.93       D
ATOM    3915  CG   ASN D 118      110.564  46.644  17.650  1.00 39.88       D
ATOM    3916  OD1  ASN D 118      110.327  47.834  17.856  1.00 42.45       D
ATOM    3917  ND2  ASN D 118      111.438  45.946  18.375  1.00 43.14       D
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ATOM   3918   C    ASN D 118   107.960  47.465  16.181  1.00 27.72      D
ATOM   3919   O    ASN D 118   108.398  47.952  15.140  1.00 26.88      D
ATOM   3920   N    ILE D 119   107.126  48.113  16.988  1.00 27.59      D
ATOM   3921   CA   ILE D 119   106.680  49.476  16.700  1.00 27.12      D
ATOM   3922   CB   ILE D 119   105.133  49.580  16.719  1.00 27.17      D
ATOM   3923   CG2  ILE D 119   104.698  50.994  16.346  1.00 26.16      D
ATOM   3924   CG1  ILE D 119   104.528  48.572  15.741  1.00 24.63      D
ATOM   3925   CD1  ILE D 119   103.026  48.423  15.877  1.00 24.19      D
ATOM   3926   C    ILE D 119   107.243  50.436  17.746  1.00 27.72      D
ATOM   3927   O    ILE D 119   107.050  50.248  18.946  1.00 26.86      D
ATOM   3928   N    THR D 120   107.951  51.460  17.291  1.00 27.54      D
ATOM   3929   CA   THR D 120   108.524  52.423  18.214  1.00 29.37      D
ATOM   3930   CB   THR D 120   110.022  52.131  18.477  1.00 32.22      D
ATOM   3931   OG1  THR D 120   110.722  52.034  17.229  1.00 35.14      D
ATOM   3932   CG2  THR D 120   110.176  50.817  19.247  1.00 35.67      D
ATOM   3933   C    THR D 120   108.369  53.826  17.668  1.00 27.95      D
ATOM   3934   O    THR D 120   108.398  54.035  16.459  1.00 29.89      D
ATOM   3935   N    TRP D 121   108.187  54.789  18.560  1.00 26.28      D
ATOM   3936   CA   TRP D 121   108.031  56.171  18.135  1.00 26.93      D
ATOM   3937   CB   TRP D 121   106.935  56.866  18.940  1.00 24.20      D
ATOM   3938   CG   TRP D 121   105.568  56.343  18.687  1.00 22.03      D
ATOM   3939   CD2  TRP D 121   104.643  56.826  17.707  1.00 20.30      D
ATOM   3940   CE2  TRP D 121   103.454  56.085  17.856  1.00 20.70      D
ATOM   3941   CE3  TRP D 121   104.705  57.817  16.717  1.00 17.15      D
ATOM   3942   CD1  TRP D 121   104.929  55.351  19.365  1.00 21.06      D
ATOM   3943   NE1  TRP D 121   103.655  55.190  18.875  1.00 22.39      D
ATOM   3944   CZ2  TRP D 121   102.332  56.305  17.057  1.00 17.25      D
ATOM   3945   CZ3  TRP D 121   103.593  58.036  15.924  1.00 17.92      D
ATOM   3946   CH2  TRP D 121   102.419  57.282  16.099  1.00 19.11      D
ATOM   3947   C    TRP D 121   109.319  56.957  18.284  1.00 26.88      D
ATOM   3948   O    TRP D 121   110.059  56.789  19.251  1.00 27.48      D
ATOM   3949   N    LEU D 122   109.572  57.830  17.321  1.00 29.82      D
ATOM   3950   CA   LEU D 122   110.764  58.658  17.343  1.00 31.91      D
ATOM   3951   CB   LEU D 122   111.664  58.331  16.144  1.00 34.65      D
ATOM   3952   CG   LEU D 122   112.391  56.977  16.112  1.00 37.28      D
ATOM   3953   CD1  LEU D 122   113.247  56.828  17.360  1.00 37.11      D
ATOM   3954   CD2  LEU D 122   111.394  55.840  16.025  1.00 39.41      D
ATOM   3955   C    LEU D 122   110.416  60.142  17.324  1.00 31.97      D
ATOM   3956   O    LEU D 122   109.619  60.593  16.503  1.00 31.46      D
ATOM   3957   N    SER D 123   111.010  60.889  18.250  1.00 31.03      D
ATOM   3958   CA   SER D 123   110.813  62.331  18.326  1.00 33.04      D
ATOM   3959   CB   SER D 123   110.312  62.745  19.712  1.00 32.42      D
ATOM   3960   OG   SER D 123   110.169  64.154  19.793  1.00 32.43      D
ATOM   3961   C    SER D 123   112.184  62.948  18.062  1.00 33.10      D
ATOM   3962   O    SER D 123   113.108  62.784  18.860  1.00 33.57      D
ATOM   3963   N    ASN D 124   112.309  63.646  16.941  1.00 33.51      D
ATOM   3964   CA   ASN D 124   113.575  64.258  16.553  1.00 36.20      D
ATOM   3965   CB   ASN D 124   113.963  65.392  17.510  1.00 34.61      D
ATOM   3966   CG   ASN D 124   112.946  66.512  17.531  1.00 34.17      D
ATOM   3967   OD1  ASN D 124   112.262  66.764  16.539  1.00 34.73      D
ATOM   3968   ND2  ASN D 124   112.850  67.202  18.660  1.00 35.34      D
ATOM   3969   C    ASN D 124   114.664  63.191  16.561  1.00 37.34      D
ATOM   3970   O    ASN D 124   115.747  63.401  17.104  1.00 37.93      D
ATOM   3971   N    GLY D 125   114.358  62.039  15.970  1.00 38.73      D
ATOM   3972   CA   GLY D 125   115.317  60.951  15.910  1.00 39.56      D
ATOM   3973   C    GLY D 125   115.457  60.131  17.183  1.00 40.55      D
ATOM   3974   O    GLY D 125   116.051  59.054  17.157  1.00 42.52      D
ATOM   3975   N    HIS D 126   114.911  60.622  18.291  1.00 40.35      D
ATOM   3976   CA   HIS D 126   115.009  59.918  19.569  1.00 41.15      D
ATOM   3977   CB   HIS D 126   115.234  60.923  20.702  1.00 43.51      D
ATOM   3978   CG   HIS D 126   116.525  61.678  20.599  1.00 47.67      D
ATOM   3979   CD2  HIS D 126   116.775  62.997  20.422  1.00 47.36      D
ATOM   3980   ND1  HIS D 126   117.757  61.064  20.694  1.00 49.39      D
ATOM   3981   CE1  HIS D 126   118.709  61.973  20.581  1.00 48.59      D
ATOM   3982   NE2  HIS D 126   118.140  63.154  20.415  1.00 48.17      D
ATOM   3983   C    HIS D 126   113.794  59.053  19.907  1.00 40.38      D
ATOM   3984   O    HIS D 126   112.648  59.458  19.706  1.00 39.87      D
ATOM   3985   N    SER D 127   114.056  57.863  20.438  1.00 39.11      D
ATOM   3986   CA   SER D 127   112.995  56.939  20.821  1.00 39.54      D
ATOM   3987   CB   SER D 127   113.592  55.592  21.232  1.00 40.04      D
ATOM   3988   OG   SER D 127   114.299  55.001  20.159  1.00 45.08      D
ATOM   3989   C    SER D 127   112.167  57.492  21.979  1.00 38.18      D
ATOM   3990   O    SER D 127   112.707  58.054  22.930  1.00 38.52      D
ATOM   3991   N    VAL D 128   110.854  57.326  21.894  1.00 36.40      D
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| ATOM | 3992 | CA  | VAL | D | 128 | 109.967 | 57.800 | 22.942 | 1.00 | 35.00 | D |
|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|---|
| ATOM | 3993 | CB  | VAL | D | 128 | 108.699 | 58.444 | 22.358 | 1.00 | 33.68 | D |
| ATOM | 3994 | CG1 | VAL | D | 128 | 107.834 | 59.001 | 23.479 | 1.00 | 32.31 | D |
| ATOM | 3995 | CG2 | VAL | D | 128 | 109.081 | 59.543 | 21.383 | 1.00 | 32.69 | D |
| ATOM | 3996 | C   | VAL | D | 128 | 109.574 | 56.608 | 23.790 | 1.00 | 34.62 | D |
| ATOM | 3997 | O   | VAL | D | 128 | 109.150 | 55.584 | 23.268 | 1.00 | 35.98 | D |
| ATOM | 3998 | N   | THR | D | 129 | 109.715 | 56.743 | 25.100 | 1.00 | 35.57 | D |
| ATOM | 3999 | CA  | THR | D | 129 | 109.393 | 55.653 | 26.007 | 1.00 | 38.21 | D |
| ATOM | 4000 | CB  | THR | D | 129 | 110.562 | 55.410 | 26.992 | 1.00 | 40.63 | D |
| ATOM | 4001 | OG1 | THR | D | 129 | 110.184 | 54.413 | 27.949 | 1.00 | 44.78 | D |
| ATOM | 4002 | CG2 | THR | D | 129 | 110.929 | 56.700 | 27.715 | 1.00 | 42.66 | D |
| ATOM | 4003 | C   | THR | D | 129 | 108.103 | 55.862 | 26.799 | 1.00 | 36.54 | D |
| ATOM | 4004 | O   | THR | D | 129 | 107.359 | 54.911 | 27.042 | 1.00 | 38.87 | D |
| ATOM | 4005 | N   | GLU | D | 130 | 107.833 | 57.101 | 27.195 | 1.00 | 33.00 | D |
| ATOM | 4006 | CA  | GLU | D | 130 | 106.631 | 57.401 | 27.963 | 1.00 | 31.03 | D |
| ATOM | 4007 | CB  | GLU | D | 130 | 106.935 | 58.453 | 29.039 | 1.00 | 33.90 | D |
| ATOM | 4008 | CG  | GLU | D | 130 | 108.067 | 58.089 | 29.987 | 1.00 | 38.08 | D |
| ATOM | 4009 | CD  | GLU | D | 130 | 107.809 | 56.788 | 30.731 | 1.00 | 43.43 | D |
| ATOM | 4010 | OE1 | GLU | D | 130 | 106.744 | 56.672 | 31.375 | 1.00 | 45.61 | D |
| ATOM | 4011 | OE2 | GLU | D | 130 | 108.671 | 55.879 | 30.675 | 1.00 | 45.67 | D |
| ATOM | 4012 | C   | GLU | D | 130 | 105.521 | 57.922 | 27.058 | 1.00 | 27.87 | D |
| ATOM | 4013 | O   | GLU | D | 130 | 105.795 | 58.527 | 26.029 | 1.00 | 24.56 | D |
| ATOM | 4014 | N   | GLY | D | 131 | 104.272 | 57.692 | 27.457 | 1.00 | 26.29 | D |
| ATOM | 4015 | CA  | GLY | D | 131 | 103.140 | 58.166 | 26.679 | 1.00 | 25.19 | D |
| ATOM | 4016 | C   | GLY | D | 131 | 102.826 | 57.304 | 25.474 | 1.00 | 24.46 | D |
| ATOM | 4017 | O   | GLY | D | 131 | 102.130 | 57.725 | 24.559 | 1.00 | 23.65 | D |
| ATOM | 4018 | N   | VAL | D | 132 | 103.349 | 56.089 | 25.476 | 1.00 | 22.83 | D |
| ATOM | 4019 | CA  | VAL | D | 132 | 103.117 | 55.169 | 24.379 | 1.00 | 23.04 | D |
| ATOM | 4020 | CB  | VAL | D | 132 | 104.448 | 54.674 | 23.784 | 1.00 | 22.91 | D |
| ATOM | 4021 | CG1 | VAL | D | 132 | 104.182 | 53.538 | 22.821 | 1.00 | 24.12 | D |
| ATOM | 4022 | CG2 | VAL | D | 132 | 105.164 | 55.816 | 23.076 | 1.00 | 22.85 | D |
| ATOM | 4023 | C   | VAL | D | 132 | 102.326 | 53.943 | 24.829 | 1.00 | 21.91 | D |
| ATOM | 4024 | O   | VAL | D | 132 | 102.535 | 53.416 | 25.917 | 1.00 | 21.27 | D |
| ATOM | 4025 | N   | SER | D | 133 | 101.412 | 53.499 | 23.979 | 1.00 | 22.08 | D |
| ATOM | 4026 | CA  | SER | D | 133 | 100.622 | 52.307 | 24.251 | 1.00 | 21.07 | D |
| ATOM | 4027 | CB  | SER | D | 133 | 99.405  | 52.637 | 25.119 | 1.00 | 21.95 | D |
| ATOM | 4028 | OG  | SER | D | 133 | 98.567  | 53.595 | 24.498 | 1.00 | 27.01 | D |
| ATOM | 4029 | C   | SER | D | 133 | 100.178 | 51.738 | 22.908 | 1.00 | 21.27 | D |
| ATOM | 4030 | O   | SER | D | 133 | 100.344 | 52.369 | 21.864 | 1.00 | 19.82 | D |
| ATOM | 4031 | N   | GLU | D | 134 | 99.627  | 50.538 | 22.926 | 1.00 | 20.29 | D |
| ATOM | 4032 | CA  | GLU | D | 134 | 99.182  | 49.938 | 21.689 | 1.00 | 24.12 | D |
| ATOM | 4033 | CB  | GLU | D | 134 | 100.370 | 49.323 | 20.932 | 1.00 | 26.01 | D |
| ATOM | 4034 | CG  | GLU | D | 134 | 100.932 | 48.045 | 21.532 | 1.00 | 30.80 | D |
| ATOM | 4035 | CD  | GLU | D | 134 | 102.080 | 47.480 | 20.704 | 1.00 | 35.43 | D |
| ATOM | 4036 | OE1 | GLU | D | 134 | 102.273 | 46.243 | 20.702 | 1.00 | 36.93 | D |
| ATOM | 4037 | OE2 | GLU | D | 134 | 102.793 | 48.278 | 20.057 | 1.00 | 37.66 | D |
| ATOM | 4038 | C   | GLU | D | 134 | 98.127  | 48.882 | 21.955 | 1.00 | 22.81 | D |
| ATOM | 4039 | O   | GLU | D | 134 | 97.968  | 48.416 | 23.081 | 1.00 | 22.94 | D |
| ATOM | 4040 | N   | THR | D | 135 | 97.400  | 48.522 | 20.908 | 1.00 | 21.95 | D |
| ATOM | 4041 | CA  | THR | D | 135 | 96.361  | 47.519 | 21.009 | 1.00 | 20.78 | D |
| ATOM | 4042 | CB  | THR | D | 135 | 95.368  | 47.625 | 19.843 | 1.00 | 20.82 | D |
| ATOM | 4043 | OG1 | THR | D | 135 | 96.032  | 47.262 | 18.623 | 1.00 | 22.24 | D |
| ATOM | 4044 | CG2 | THR | D | 135 | 94.833  | 49.046 | 19.721 | 1.00 | 18.01 | D |
| ATOM | 4045 | C   | THR | D | 135 | 97.037  | 46.168 | 20.890 | 1.00 | 20.80 | D |
| ATOM | 4046 | O   | THR | D | 135 | 98.259  | 46.084 | 20.742 | 1.00 | 21.08 | D |
| ATOM | 4047 | N   | SER | D | 136 | 96.234  | 45.116 | 20.972 | 1.00 | 19.11 | D |
| ATOM | 4048 | CA  | SER | D | 136 | 96.728  | 43.764 | 20.790 | 1.00 | 16.93 | D |
| ATOM | 4049 | CB  | SER | D | 136 | 95.769  | 42.755 | 21.428 | 1.00 | 19.17 | D |
| ATOM | 4050 | OG  | SER | D | 136 | 95.656  | 42.951 | 22.831 | 1.00 | 23.01 | D |
| ATOM | 4051 | C   | SER | D | 136 | 96.665  | 43.635 | 19.267 | 1.00 | 15.30 | D |
| ATOM | 4052 | O   | SER | D | 136 | 96.325  | 44.592 | 18.580 | 1.00 | 13.19 | D |
| ATOM | 4053 | N   | PHE | D | 137 | 97.002  | 42.472 | 18.733 | 1.00 | 16.43 | D |
| ATOM | 4054 | CA  | PHE | D | 137 | 96.896  | 42.267 | 17.294 | 1.00 | 16.20 | D |
| ATOM | 4055 | CB  | PHE | D | 137 | 97.652  | 41.001 | 16.874 | 1.00 | 15.86 | D |
| ATOM | 4056 | CG  | PHE | D | 137 | 99.138  | 41.146 | 16.879 | 1.00 | 17.29 | D |
| ATOM | 4057 | CD1 | PHE | D | 137 | 99.792  | 41.775 | 15.823 | 1.00 | 20.23 | D |
| ATOM | 4058 | CD2 | PHE | D | 137 | 99.894  | 40.644 | 17.932 | 1.00 | 17.79 | D |
| ATOM | 4059 | CE1 | PHE | D | 137 | 101.187 | 41.900 | 15.815 | 1.00 | 21.20 | D |
| ATOM | 4060 | CE2 | PHE | D | 137 | 101.291 | 40.762 | 17.936 | 1.00 | 19.39 | D |
| ATOM | 4061 | CZ  | PHE | D | 137 | 101.935 | 41.392 | 16.874 | 1.00 | 19.70 | D |
| ATOM | 4062 | C   | PHE | D | 137 | 95.402  | 42.056 | 17.025 | 1.00 | 16.08 | D |
| ATOM | 4063 | O   | PHE | D | 137 | 94.823  | 41.121 | 17.556 | 1.00 | 15.19 | D |
| ATOM | 4064 | N   | LEU | D | 138 | 94.786  | 42.925 | 16.227 | 1.00 | 19.23 | D |
| ATOM | 4065 | CA  | LEU | D | 138 | 93.367  | 42.797 | 15.882 | 1.00 | 21.12 | D |

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| ATOM | 4066 | CB | LEU | D | 138 | 92.722 | 44.175 | 15.678 | 1.00 | 21.40 | D |
|------|------|------|------|---|------|--------|--------|--------|------|-------|---|
| ATOM | 4067 | CG | LEU | D | 138 | 92.452 | 45.087 | 16.881 | 1.00 | 22.42 | D |
| ATOM | 4068 | CD1 | LEU | D | 138 | 91.889 | 44.277 | 18.032 | 1.00 | 23.38 | D |
| ATOM | 4069 | CD2 | LEU | D | 138 | 93.732 | 45.764 | 17.301 | 1.00 | 28.68 | D |
| ATOM | 4070 | C | LEU | D | 138 | 93.230 | 41.982 | 14.593 | 1.00 | 20.56 | D |
| ATOM | 4071 | O | LEU | D | 138 | 93.919 | 42.244 | 13.615 | 1.00 | 22.27 | D |
| ATOM | 4072 | N | SER | D | 139 | 92.326 | 41.013 | 14.586 | 1.00 | 20.44 | D |
| ATOM | 4073 | CA | SER | D | 139 | 92.143 | 40.142 | 13.427 | 1.00 | 19.23 | D |
| ATOM | 4074 | CB | SER | D | 139 | 91.222 | 38.986 | 13.788 | 1.00 | 19.74 | D |
| ATOM | 4075 | OG | SER | D | 139 | 89.888 | 39.443 | 13.861 | 1.00 | 21.32 | D |
| ATOM | 4076 | C | SER | D | 139 | 91.594 | 40.802 | 12.168 | 1.00 | 19.43 | D |
| ATOM | 4077 | O | SER | D | 139 | 91.028 | 41.893 | 12.210 | 1.00 | 19.49 | D |
| ATOM | 4078 | N | LYS | D | 140 | 91.755 | 40.102 | 11.050 | 1.00 | 18.62 | D |
| ATOM | 4079 | CA | LYS | D | 140 | 91.276 | 40.553 | 9.749 | 1.00 | 19.20 | D |
| ATOM | 4080 | CB | LYS | D | 140 | 92.437 | 41.058 | 8.895 | 1.00 | 18.92 | D |
| ATOM | 4081 | CG | LYS | D | 140 | 93.286 | 42.126 | 9.554 | 1.00 | 19.38 | D |
| ATOM | 4082 | CD | LYS | D | 140 | 93.254 | 43.393 | 8.758 | 1.00 | 20.95 | D |
| ATOM | 4083 | CE | LYS | D | 140 | 93.833 | 43.195 | 7.377 | 1.00 | 18.23 | D |
| ATOM | 4084 | NZ | LYS | D | 140 | 93.743 | 44.457 | 6.617 | 1.00 | 20.40 | D |
| ATOM | 4085 | C | LYS | D | 140 | 90.660 | 39.339 | 9.068 | 1.00 | 19.16 | D |
| ATOM | 4086 | O | LYS | D | 140 | 91.091 | 38.217 | 9.312 | 1.00 | 19.77 | D |
| ATOM | 4087 | N | SER | D | 141 | 89.670 | 39.552 | 8.207 | 1.00 | 21.60 | D |
| ATOM | 4088 | CA | SER | D | 141 | 89.030 | 38.438 | 7.507 | 1.00 | 23.19 | D |
| ATOM | 4089 | CB | SER | D | 141 | 87.859 | 38.948 | 6.653 | 1.00 | 24.88 | D |
| ATOM | 4090 | OG | SER | D | 141 | 88.288 | 39.858 | 5.655 | 1.00 | 28.69 | D |
| ATOM | 4091 | C | SER | D | 141 | 89.989 | 37.605 | 6.636 | 1.00 | 23.26 | D |
| ATOM | 4092 | O | SER | D | 141 | 89.692 | 36.454 | 6.327 | 1.00 | 23.33 | D |
| ATOM | 4093 | N | ASP | D | 142 | 91.137 | 38.159 | 6.251 | 1.00 | 21.38 | D |
| ATOM | 4094 | CA | ASP | D | 142 | 92.075 | 37.387 | 5.429 | 1.00 | 22.54 | D |
| ATOM | 4095 | CB | ASP | D | 142 | 92.834 | 38.303 | 4.466 | 1.00 | 25.84 | D |
| ATOM | 4096 | CG | ASP | D | 142 | 93.943 | 39.064 | 5.143 | 1.00 | 29.78 | D |
| ATOM | 4097 | OD1 | ASP | D | 142 | 93.760 | 39.486 | 6.309 | 1.00 | 31.16 | D |
| ATOM | 4098 | OD2 | ASP | D | 142 | 94.997 | 39.246 | 4.500 | 1.00 | 34.64 | D |
| ATOM | 4099 | C | ASP | D | 142 | 93.045 | 36.637 | 6.336 | 1.00 | 22.89 | D |
| ATOM | 4100 | O | ASP | D | 142 | 94.027 | 36.037 | 5.883 | 1.00 | 20.54 | D |
| ATOM | 4101 | N | HIS | D | 143 | 92.753 | 36.700 | 7.632 | 1.00 | 21.06 | D |
| ATOM | 4102 | CA | HIS | D | 143 | 93.522 | 36.020 | 8.659 | 1.00 | 19.58 | D |
| ATOM | 4103 | CB | HIS | D | 143 | 93.628 | 34.534 | 8.317 | 1.00 | 19.03 | D |
| ATOM | 4104 | CG | HIS | D | 143 | 92.295 | 33.892 | 8.104 | 1.00 | 23.00 | D |
| ATOM | 4105 | CD2 | HIS | D | 143 | 91.827 | 33.108 | 7.104 | 1.00 | 24.78 | D |
| ATOM | 4106 | ND1 | HIS | D | 143 | 91.237 | 34.087 | 8.967 | 1.00 | 21.97 | D |
| ATOM | 4107 | CE1 | HIS | D | 143 | 90.174 | 33.455 | 8.505 | 1.00 | 24.67 | D |
| ATOM | 4108 | NE2 | HIS | D | 143 | 90.504 | 32.853 | 7.375 | 1.00 | 24.72 | D |
| ATOM | 4109 | C | HIS | D | 143 | 94.878 | 36.602 | 8.986 | 1.00 | 20.11 | D |
| ATOM | 4110 | O | HIS | D | 143 | 95.691 | 35.962 | 9.654 | 1.00 | 21.09 | D |
| ATOM | 4111 | N | SER | D | 144 | 95.118 | 37.820 | 8.514 | 1.00 | 21.24 | D |
| ATOM | 4112 | CA | SER | D | 144 | 96.352 | 38.525 | 8.826 | 1.00 | 21.79 | D |
| ATOM | 4113 | CB | SER | D | 144 | 96.834 | 39.353 | 7.627 | 1.00 | 20.33 | D |
| ATOM | 4114 | OG | SER | D | 144 | 96.047 | 40.511 | 7.434 | 1.00 | 24.32 | D |
| ATOM | 4115 | C | SER | D | 144 | 95.940 | 39.440 | 9.990 | 1.00 | 21.43 | D |
| ATOM | 4116 | O | SER | D | 144 | 94.830 | 39.317 | 10.504 | 1.00 | 20.74 | D |
| ATOM | 4117 | N | PHE | D | 145 | 96.809 | 40.352 | 10.412 | 1.00 | 21.56 | D |
| ATOM | 4118 | CA | PHE | D | 145 | 96.463 | 41.235 | 11.523 | 1.00 | 22.54 | D |
| ATOM | 4119 | CB | PHE | D | 145 | 97.156 | 40.791 | 12.817 | 1.00 | 22.63 | D |
| ATOM | 4120 | CG | PHE | D | 145 | 96.896 | 39.368 | 13.200 | 1.00 | 25.73 | D |
| ATOM | 4121 | CD1 | PHE | D | 145 | 97.565 | 38.329 | 12.562 | 1.00 | 26.67 | D |
| ATOM | 4122 | CD2 | PHE | D | 145 | 95.987 | 39.063 | 14.207 | 1.00 | 23.65 | D |
| ATOM | 4123 | CE1 | PHE | D | 145 | 97.333 | 37.004 | 12.921 | 1.00 | 27.30 | D |
| ATOM | 4124 | CE2 | PHE | D | 145 | 95.750 | 37.746 | 14.572 | 1.00 | 25.43 | D |
| ATOM | 4125 | CZ | PHE | D | 145 | 96.426 | 36.713 | 13.926 | 1.00 | 24.90 | D |
| ATOM | 4126 | C | PHE | D | 145 | 96.850 | 42.687 | 11.299 | 1.00 | 22.51 | D |
| ATOM | 4127 | O | PHE | D | 145 | 97.540 | 43.028 | 10.339 | 1.00 | 23.97 | D |
| ATOM | 4128 | N | PHE | D | 146 | 96.371 | 43.540 | 12.198 | 1.00 | 20.96 | D |
| ATOM | 4129 | CA | PHE | D | 146 | 96.729 | 44.946 | 12.190 | 1.00 | 19.68 | D |
| ATOM | 4130 | CB | PHE | D | 146 | 95.696 | 45.817 | 11.439 | 1.00 | 17.70 | D |
| ATOM | 4131 | CG | PHE | D | 146 | 94.392 | 46.041 | 12.159 | 1.00 | 15.76 | D |
| ATOM | 4132 | CD1 | PHE | D | 146 | 94.201 | 47.173 | 12.948 | 1.00 | 16.08 | D |
| ATOM | 4133 | CD2 | PHE | D | 146 | 93.321 | 45.170 | 11.976 | 1.00 | 14.70 | D |
| ATOM | 4134 | CE1 | PHE | D | 146 | 92.961 | 47.442 | 13.543 | 1.00 | 13.47 | D |
| ATOM | 4135 | CE2 | PHE | D | 146 | 92.080 | 45.426 | 12.563 | 1.00 | 15.43 | D |
| ATOM | 4136 | CZ | PHE | D | 146 | 91.900 | 46.567 | 13.350 | 1.00 | 14.68 | D |
| ATOM | 4137 | C | PHE | D | 146 | 96.893 | 45.335 | 13.654 | 1.00 | 19.66 | D |
| ATOM | 4138 | O | PHE | D | 146 | 96.373 | 44.672 | 14.551 | 1.00 | 19.92 | D |
| ATOM | 4139 | N | LYS | D | 147 | 97.666 | 46.379 | 13.901 | 1.00 | 20.23 | D |

| ATOM | 4140 | CA | LYS | D | 147 | 97.910 | 46.817 | 15.260 | 1.00 | 19.84 | D |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 4141 | CB | LYS | D | 147 | 99.184 | 46.148 | 15.796 | 1.00 | 21.50 | D |
| ATOM | 4142 | CG | LYS | D | 147 | 99.651 | 46.679 | 17.134 | 1.00 | 24.87 | D |
| ATOM | 4143 | CD | LYS | D | 147 | 100.764 | 45.832 | 17.724 | 1.00 | 27.18 | D |
| ATOM | 4144 | CE | LYS | D | 147 | 100.220 | 44.515 | 18.253 | 1.00 | 31.41 | D |
| ATOM | 4145 | NZ | LYS | D | 147 | 101.086 | 43.984 | 19.341 | 1.00 | 32.97 | D |
| ATOM | 4146 | C | LYS | D | 147 | 98.038 | 48.324 | 15.274 | 1.00 | 18.69 | D |
| ATOM | 4147 | O | LYS | D | 147 | 98.603 | 48.914 | 14.352 | 1.00 | 20.14 | D |
| ATOM | 4148 | N | ILE | D | 148 | 97.497 | 48.944 | 16.314 | 1.00 | 18.22 | D |
| ATOM | 4149 | CA | ILE | D | 148 | 97.530 | 50.387 | 16.446 | 1.00 | 18.25 | D |
| ATOM | 4150 | CB | ILE | D | 148 | 96.092 | 50.942 | 16.548 | 1.00 | 20.80 | D |
| ATOM | 4151 | CG2 | ILE | D | 148 | 96.113 | 52.459 | 16.659 | 1.00 | 22.44 | D |
| ATOM | 4152 | CG1 | ILE | D | 148 | 95.308 | 50.533 | 15.292 | 1.00 | 23.89 | D |
| ATOM | 4153 | CD1 | ILE | D | 148 | 93.840 | 50.858 | 15.314 | 1.00 | 24.42 | D |
| ATOM | 4154 | C | ILE | D | 148 | 98.369 | 50.816 | 17.646 | 1.00 | 19.71 | D |
| ATOM | 4155 | O | ILE | D | 148 | 98.213 | 50.294 | 18.757 | 1.00 | 17.77 | D |
| ATOM | 4156 | N | SER | D | 149 | 99.284 | 51.753 | 17.395 | 1.00 | 19.08 | D |
| ATOM | 4157 | CA | SER | D | 149 | 100.173 | 52.278 | 18.424 | 1.00 | 18.19 | D |
| ATOM | 4158 | CB | SER | D | 149 | 101.633 | 52.137 | 17.991 | 1.00 | 18.51 | D |
| ATOM | 4159 | OG | SER | D | 149 | 102.518 | 52.492 | 19.040 | 1.00 | 19.49 | D |
| ATOM | 4160 | C | SER | D | 149 | 99.839 | 53.744 | 18.646 | 1.00 | 18.14 | D |
| ATOM | 4161 | O | SER | D | 149 | 99.591 | 54.490 | 17.693 | 1.00 | 18.17 | D |
| ATOM | 4162 | N | TYR | D | 150 | 99.843 | 54.155 | 19.905 | 1.00 | 16.95 | D |
| ATOM | 4163 | CA | TYR | D | 150 | 99.503 | 55.524 | 20.261 | 1.00 | 16.12 | D |
| ATOM | 4164 | CB | TYR | D | 150 | 98.310 | 55.524 | 21.213 | 1.00 | 15.57 | D |
| ATOM | 4165 | CG | TYR | D | 150 | 97.116 | 54.750 | 20.701 | 1.00 | 16.81 | D |
| ATOM | 4166 | CD1 | TYR | D | 150 | 96.291 | 55.276 | 19.709 | 1.00 | 14.33 | D |
| ATOM | 4167 | CE1 | TYR | D | 150 | 95.197 | 54.554 | 19.222 | 1.00 | 17.50 | D |
| ATOM | 4168 | CD2 | TYR | D | 150 | 96.819 | 53.486 | 21.199 | 1.00 | 15.90 | D |
| ATOM | 4169 | CE2 | TYR | D | 150 | 95.731 | 52.760 | 20.719 | 1.00 | 18.41 | D |
| ATOM | 4170 | CZ | TYR | D | 150 | 94.928 | 53.297 | 19.732 | 1.00 | 16.27 | D |
| ATOM | 4171 | OH | TYR | D | 150 | 93.868 | 52.574 | 19.244 | 1.00 | 20.03 | D |
| ATOM | 4172 | C | TYR | D | 150 | 100.650 | 56.266 | 20.922 | 1.00 | 16.35 | D |
| ATOM | 4173 | O | TYR | D | 150 | 101.438 | 55.690 | 21.669 | 1.00 | 16.95 | D |
| ATOM | 4174 | N | LEU | D | 151 | 100.732 | 57.558 | 20.643 | 1.00 | 16.64 | D |
| ATOM | 4175 | CA | LEU | D | 151 | 101.760 | 58.396 | 21.227 | 1.00 | 16.50 | D |
| ATOM | 4176 | CB | LEU | D | 151 | 102.849 | 58.705 | 20.203 | 1.00 | 15.48 | D |
| ATOM | 4177 | CG | LEU | D | 151 | 103.806 | 59.825 | 20.639 | 1.00 | 17.55 | D |
| ATOM | 4178 | CD1 | LEU | D | 151 | 104.641 | 59.374 | 21.834 | 1.00 | 16.60 | D |
| ATOM | 4179 | CD2 | LEU | D | 151 | 104.702 | 60.213 | 19.476 | 1.00 | 16.11 | D |
| ATOM | 4180 | C | LEU | D | 151 | 101.140 | 59.701 | 21.693 | 1.00 | 17.56 | D |
| ATOM | 4181 | O | LEU | D | 151 | 100.577 | 60.440 | 20.888 | 1.00 | 17.18 | D |
| ATOM | 4182 | N | THR | D | 152 | 101.233 | 59.997 | 22.983 | 1.00 | 16.14 | D |
| ATOM | 4183 | CA | THR | D | 152 | 100.690 | 61.259 | 23.448 | 1.00 | 19.47 | D |
| ATOM | 4184 | CB | THR | D | 152 | 100.359 | 61.248 | 24.966 | 1.00 | 21.24 | D |
| ATOM | 4185 | OG1 | THR | D | 152 | 101.517 | 60.871 | 25.725 | 1.00 | 25.03 | D |
| ATOM | 4186 | CG2 | THR | D | 152 | 99.214 | 60.281 | 25.247 | 1.00 | 20.79 | D |
| ATOM | 4187 | C | THR | D | 152 | 101.717 | 62.345 | 23.151 | 1.00 | 19.82 | D |
| ATOM | 4188 | O | THR | D | 152 | 102.921 | 62.113 | 23.218 | 1.00 | 21.31 | D |
| ATOM | 4189 | N | LEU | D | 153 | 101.241 | 63.523 | 22.781 | 1.00 | 20.76 | D |
| ATOM | 4190 | CA | LEU | D | 153 | 102.143 | 64.617 | 22.488 | 1.00 | 24.15 | D |
| ATOM | 4191 | CB | LEU | D | 153 | 102.760 | 64.450 | 21.089 | 1.00 | 25.45 | D |
| ATOM | 4192 | CG | LEU | D | 153 | 101.959 | 64.575 | 19.785 | 1.00 | 27.17 | D |
| ATOM | 4193 | CD1 | LEU | D | 153 | 100.520 | 64.101 | 19.986 | 1.00 | 27.83 | D |
| ATOM | 4194 | CD2 | LEU | D | 153 | 101.982 | 66.015 | 19.319 | 1.00 | 27.38 | D |
| ATOM | 4195 | C | LEU | D | 153 | 101.440 | 65.952 | 22.601 | 1.00 | 25.73 | D |
| ATOM | 4196 | O | LEU | D | 153 | 100.208 | 66.028 | 22.681 | 1.00 | 26.55 | D |
| ATOM | 4197 | N | LEU | D | 154 | 102.251 | 67.000 | 22.640 | 1.00 | 26.77 | D |
| ATOM | 4198 | CA | LEU | D | 154 | 101.781 | 68.369 | 22.734 | 1.00 | 26.34 | D |
| ATOM | 4199 | CB | LEU | D | 154 | 102.298 | 69.027 | 24.019 | 1.00 | 25.08 | D |
| ATOM | 4200 | CG | LEU | D | 154 | 101.877 | 70.478 | 24.288 | 1.00 | 26.28 | D |
| ATOM | 4201 | CD1 | LEU | D | 154 | 100.377 | 70.531 | 24.570 | 1.00 | 24.44 | D |
| ATOM | 4202 | CD2 | LEU | D | 154 | 102.667 | 71.031 | 25.477 | 1.00 | 23.08 | D |
| ATOM | 4203 | C | LEU | D | 154 | 102.374 | 69.063 | 21.522 | 1.00 | 28.41 | D |
| ATOM | 4204 | O | LEU | D | 154 | 103.577 | 69.327 | 21.468 | 1.00 | 27.19 | D |
| ATOM | 4205 | N | PRO | D | 155 | 101.534 | 69.351 | 20.523 | 1.00 | 30.32 | D |
| ATOM | 4206 | CD | PRO | D | 155 | 100.109 | 68.979 | 20.453 | 1.00 | 30.25 | D |
| ATOM | 4207 | CA | PRO | D | 155 | 101.965 | 70.014 | 19.294 | 1.00 | 31.71 | D |
| ATOM | 4208 | CB | PRO | D | 155 | 100.667 | 70.160 | 18.510 | 1.00 | 31.92 | D |
| ATOM | 4209 | CG | PRO | D | 155 | 99.861 | 68.968 | 18.963 | 1.00 | 31.51 | D |
| ATOM | 4210 | C | PRO | D | 155 | 102.663 | 71.354 | 19.508 | 1.00 | 35.12 | D |
| ATOM | 4211 | O | PRO | D | 155 | 102.110 | 72.275 | 20.112 | 1.00 | 35.64 | D |
| ATOM | 4212 | N | SER | D | 156 | 103.893 | 71.436 | 19.014 | 1.00 | 39.00 | D |
| ATOM | 4213 | CA | SER | D | 156 | 104.706 | 72.643 | 19.083 | 1.00 | 42.94 | D |

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ATOM   4214  CB   SER D 156      105.819  72.492  20.121  1.00 43.03      D
ATOM   4215  OG   SER D 156      105.288  72.385  21.430  1.00 45.30      D
ATOM   4216  C    SER D 156      105.311  72.763  17.694  1.00 46.03      D
ATOM   4217  O    SER D 156      104.875  72.084  16.770  1.00 47.06      D
ATOM   4218  N    ALA D 157      106.316  73.609  17.534  1.00 49.61      D
ATOM   4219  CA   ALA D 157      106.931  73.756  16.222  1.00 51.03      D
ATOM   4220  CB   ALA D 157      106.977  75.231  15.828  1.00 51.20      D
ATOM   4221  C    ALA D 157      108.334  73.163  16.195  1.00 51.50      D
ATOM   4222  O    ALA D 157      108.985  73.147  15.150  1.00 52.20      D
ATOM   4223  N    GLU D 158      108.797  72.669  17.339  1.00 52.37      D
ATOM   4224  CA   GLU D 158      110.141  72.103  17.411  1.00 53.43      D
ATOM   4225  CB   GLU D 158      110.946  72.785  18.524  1.00 57.17      D
ATOM   4226  CG   GLU D 158      110.401  72.570  19.934  1.00 61.50      D
ATOM   4227  CD   GLU D 158      109.278  73.529  20.291  1.00 63.75      D
ATOM   4228  OE1  GLU D 158      108.757  73.431  21.425  1.00 63.56      D
ATOM   4229  OE2  GLU D 158      108.922  74.381  19.445  1.00 65.17      D
ATOM   4230  C    GLU D 158      110.190  70.592  17.614  1.00 51.03      D
ATOM   4231  O    GLU D 158      111.103  70.084  18.265  1.00 51.07      D
ATOM   4232  N    GLU D 159      109.219  69.876  17.057  1.00 47.47      D
ATOM   4233  CA   GLU D 159      109.185  68.425  17.193  1.00 46.22      D
ATOM   4234  CB   GLU D 159      108.337  68.013  18.406  1.00 47.11      D
ATOM   4235  CG   GLU D 159      109.127  67.692  19.671  1.00 48.53      D
ATOM   4236  CD   GLU D 159      108.268  67.042  20.751  1.00 50.37      D
ATOM   4237  OE1  GLU D 159      107.319  67.694  21.238  1.00 50.39      D
ATOM   4238  OE2  GLU D 159      108.537  65.873  21.112  1.00 50.03      D
ATOM   4239  C    GLU D 159      108.641  67.714  15.960  1.00 43.84      D
ATOM   4240  O    GLU D 159      107.515  67.974  15.535  1.00 44.12      D
ATOM   4241  N    SER D 160      109.443  66.825  15.380  1.00 39.56      D
ATOM   4242  CA   SER D 160      108.993  66.054  14.229  1.00 37.29      D
ATOM   4243  CB   SER D 160      109.971  66.172  13.055  1.00 37.41      D
ATOM   4244  OG   SER D 160      111.070  65.298  13.206  1.00 41.72      D
ATOM   4245  C    SER D 160      108.933  64.615  14.734  1.00 35.08      D
ATOM   4246  O    SER D 160      109.754  64.207  15.557  1.00 33.66      D
ATOM   4247  N    TYR D 161      107.961  63.846  14.260  1.00 32.11      D
ATOM   4248  CA   TYR D 161      107.828  62.478  14.728  1.00 29.69      D
ATOM   4249  CB   TYR D 161      106.550  62.315  15.547  1.00 29.62      D
ATOM   4250  CG   TYR D 161      106.347  63.349  16.620  1.00 29.33      D
ATOM   4251  CD1  TYR D 161      105.761  64.577  16.327  1.00 31.31      D
ATOM   4252  CE1  TYR D 161      105.513  65.515  17.329  1.00 32.70      D
ATOM   4253  CD2  TYR D 161      106.695  63.085  17.937  1.00 30.13      D
ATOM   4254  CE2  TYR D 161      106.457  64.013  18.947  1.00 30.43      D
ATOM   4255  CZ   TYR D 161      105.863  65.223  18.638  1.00 31.92      D
ATOM   4256  OH   TYR D 161      105.592  66.128  19.643  1.00 35.12      D
ATOM   4257  C    TYR D 161      107.820  61.441  13.627  1.00 29.60      D
ATOM   4258  O    TYR D 161      107.493  61.728  12.473  1.00 29.45      D
ATOM   4259  N    ASP D 162      108.172  60.221  14.005  1.00 29.35      D
ATOM   4260  CA   ASP D 162      108.201  59.109  13.075  1.00 30.15      D
ATOM   4261  CB   ASP D 162      109.618  58.863  12.548  1.00 34.90      D
ATOM   4262  CG   ASP D 162      110.154  60.016  11.733  1.00 37.70      D
ATOM   4263  OD1  ASP D 162      109.669  60.218  10.597  1.00 40.13      D
ATOM   4264  OD2  ASP D 162      111.061  60.716  12.235  1.00 38.68      D
ATOM   4265  C    ASP D 162      107.759  57.851  13.784  1.00 29.84      D
ATOM   4266  O    ASP D 162      108.010  57.672  14.978  1.00 26.72      D
ATOM   4267  N    CYS D 163      107.088  56.984  13.039  1.00 29.31      D
ATOM   4268  CA   CYS D 163      106.684  55.700  13.569  1.00 29.59      D
ATOM   4269  C    CYS D 163      107.689  54.769  12.902  1.00 28.04      D
ATOM   4270  O    CYS D 163      107.822  54.772  11.685  1.00 26.22      D
ATOM   4271  CB   CYS D 163      105.265  55.326  13.134  1.00 29.11      D
ATOM   4272  SG   CYS D 163      104.703  53.760  13.878  1.00 34.32      D
ATOM   4273  N    LYS D 164      108.417  54.001  13.699  1.00 29.03      D
ATOM   4274  CA   LYS D 164      109.404  53.072  13.161  1.00 29.67      D
ATOM   4275  CB   LYS D 164      110.730  53.238  13.911  1.00 32.54      D
ATOM   4276  CG   LYS D 164      111.874  52.352  13.416  1.00 34.76      D
ATOM   4277  CD   LYS D 164      113.109  52.528  14.297  1.00 34.79      D
ATOM   4278  CE   LYS D 164      114.254  51.630  13.850  1.00 38.29      D
ATOM   4279  NZ   LYS D 164      115.425  51.702  14.775  1.00 36.58      D
ATOM   4280  C    LYS D 164      108.863  51.651  13.322  1.00 28.94      D
ATOM   4281  O    LYS D 164      108.642  51.189  14.443  1.00 29.32      D
ATOM   4282  N    VAL D 165      108.632  50.974  12.197  1.00 27.33      D
ATOM   4283  CA   VAL D 165      108.100  49.618  12.212  1.00 26.58      D
ATOM   4284  CB   VAL D 165      106.797  49.516  11.359  1.00 27.12      D
ATOM   4285  CG1  VAL D 165      106.199  48.122  11.462  1.00 25.56      D
ATOM   4286  CG2  VAL D 165      105.787  50.544  11.827  1.00 27.97      D
ATOM   4287  C    VAL D 165      109.113  48.600  11.690  1.00 26.91      D
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| ATOM | 4288 | O   | VAL D 165 | 109.621 | 48.720 | 10.583 | 1.00 | 25.56 | D |
|------|------|-----|-----------|---------|--------|--------|------|-------|---|
| ATOM | 4289 | N   | GLU D 166 | 109.414 | 47.606 | 12.513 | 1.00 | 28.75 | D |
| ATOM | 4290 | CA  | GLU D 166 | 110.338 | 46.544 | 12.139 | 1.00 | 30.67 | D |
| ATOM | 4291 | CB  | GLU D 166 | 111.445 | 46.410 | 13.194 | 1.00 | 33.57 | D |
| ATOM | 4292 | CG  | GLU D 166 | 112.452 | 47.565 | 13.142 | 1.00 | 41.68 | D |
| ATOM | 4293 | CD  | GLU D 166 | 113.506 | 47.526 | 14.244 | 1.00 | 46.12 | D |
| ATOM | 4294 | OE1 | GLU D 166 | 114.482 | 48.304 | 14.146 | 1.00 | 49.01 | D |
| ATOM | 4295 | OE2 | GLU D 166 | 113.363 | 46.736 | 15.206 | 1.00 | 49.40 | D |
| ATOM | 4296 | C   | GLU D 166 | 109.543 | 45.243 | 12.008 | 1.00 | 30.18 | D |
| ATOM | 4297 | O   | GLU D 166 | 108.737 | 44.900 | 12.878 | 1.00 | 28.51 | D |
| ATOM | 4298 | N   | HIS D 167 | 109.759 | 44.535 | 10.907 | 1.00 | 29.48 | D |
| ATOM | 4299 | CA  | HIS D 167 | 109.056 | 43.281 | 10.648 | 1.00 | 30.29 | D |
| ATOM | 4300 | CB  | HIS D 167 | 107.686 | 43.569 | 10.025 | 1.00 | 29.56 | D |
| ATOM | 4301 | CG  | HIS D 167 | 106.808 | 42.363 |  9.903 | 1.00 | 30.02 | D |
| ATOM | 4302 | CD2 | HIS D 167 | 106.562 | 41.541 |  8.856 | 1.00 | 29.91 | D |
| ATOM | 4303 | ND1 | HIS D 167 | 106.068 | 41.871 | 10.957 | 1.00 | 31.27 | D |
| ATOM | 4304 | CE1 | HIS D 167 | 105.404 | 40.798 | 10.564 | 1.00 | 28.43 | D |
| ATOM | 4305 | NE2 | HIS D 167 | 105.687 | 40.576 |  9.293 | 1.00 | 28.97 | D |
| ATOM | 4306 | C   | HIS D 167 | 109.886 | 42.440 |  9.684 | 1.00 | 30.36 | D |
| ATOM | 4307 | O   | HIS D 167 | 110.607 | 42.976 |  8.842 | 1.00 | 30.66 | D |
| ATOM | 4308 | N   | TRP D 168 | 109.775 | 41.122 |  9.801 | 1.00 | 31.13 | D |
| ATOM | 4309 | CA  | TRP D 168 | 110.521 | 40.219 |  8.930 | 1.00 | 32.08 | D |
| ATOM | 4310 | CB  | TRP D 168 | 110.270 | 38.765 |  9.336 | 1.00 | 28.28 | D |
| ATOM | 4311 | CG  | TRP D 168 | 110.665 | 38.475 | 10.739 | 1.00 | 26.36 | D |
| ATOM | 4312 | CD2 | TRP D 168 | 110.031 | 37.556 | 11.635 | 1.00 | 25.51 | D |
| ATOM | 4313 | CE2 | TRP D 168 | 110.759 | 37.578 | 12.842 | 1.00 | 26.35 | D |
| ATOM | 4314 | CE3 | TRP D 168 | 108.916 | 36.715 | 11.534 | 1.00 | 24.88 | D |
| ATOM | 4315 | CD1 | TRP D 168 | 111.721 | 39.004 | 11.416 | 1.00 | 27.27 | D |
| ATOM | 4316 | NE1 | TRP D 168 | 111.786 | 38.471 | 12.682 | 1.00 | 28.25 | D |
| ATOM | 4317 | CZ2 | TRP D 168 | 110.412 | 36.791 | 13.943 | 1.00 | 27.00 | D |
| ATOM | 4318 | CZ3 | TRP D 168 | 108.568 | 35.932 | 12.628 | 1.00 | 25.90 | D |
| ATOM | 4319 | CH2 | TRP D 168 | 109.315 | 35.976 | 13.817 | 1.00 | 26.65 | D |
| ATOM | 4320 | C   | TRP D 168 | 110.180 | 40.403 |  7.452 | 1.00 | 33.22 | D |
| ATOM | 4321 | O   | TRP D 168 | 111.011 | 40.139 |  6.582 | 1.00 | 33.90 | D |
| ATOM | 4322 | N   | GLY D 169 | 108.959 | 40.853 |  7.174 | 1.00 | 34.75 | D |
| ATOM | 4323 | CA  | GLY D 169 | 108.533 | 41.060 |  5.797 | 1.00 | 36.14 | D |
| ATOM | 4324 | C   | GLY D 169 | 109.056 | 42.359 |  5.215 | 1.00 | 37.80 | D |
| ATOM | 4325 | O   | GLY D 169 | 108.635 | 42.796 |  4.139 | 1.00 | 36.95 | D |
| ATOM | 4326 | N   | LEU D 170 | 109.979 | 42.981 |  5.938 | 1.00 | 38.89 | D |
| ATOM | 4327 | CA  | LEU D 170 | 110.578 | 44.234 |  5.509 | 1.00 | 40.79 | D |
| ATOM | 4328 | CB  | LEU D 170 | 110.212 | 45.356 |  6.480 | 1.00 | 39.77 | D |
| ATOM | 4329 | CG  | LEU D 170 | 108.745 | 45.765 |  6.581 | 1.00 | 39.57 | D |
| ATOM | 4330 | CD1 | LEU D 170 | 108.592 | 46.809 |  7.671 | 1.00 | 38.10 | D |
| ATOM | 4331 | CD2 | LEU D 170 | 108.267 | 46.308 |  5.243 | 1.00 | 39.58 | D |
| ATOM | 4332 | C   | LEU D 170 | 112.092 | 44.085 |  5.465 | 1.00 | 42.12 | D |
| ATOM | 4333 | O   | LEU D 170 | 112.688 | 43.506 |  6.370 | 1.00 | 41.54 | D |
| ATOM | 4334 | N   | ASP D 171 | 112.706 | 44.613 |  4.411 | 1.00 | 45.36 | D |
| ATOM | 4335 | CA  | ASP D 171 | 114.158 | 44.559 |  4.252 | 1.00 | 48.35 | D |
| ATOM | 4336 | CB  | ASP D 171 | 114.539 | 44.947 |  2.820 | 1.00 | 50.69 | D |
| ATOM | 4337 | CG  | ASP D 171 | 113.467 | 45.775 |  2.137 | 1.00 | 52.75 | D |
| ATOM | 4338 | OD1 | ASP D 171 | 113.076 | 46.827 |  2.689 | 1.00 | 54.19 | D |
| ATOM | 4339 | OD2 | ASP D 171 | 113.012 | 45.372 |  1.046 | 1.00 | 54.32 | D |
| ATOM | 4340 | C   | ASP D 171 | 114.849 | 45.485 |  5.255 | 1.00 | 48.43 | D |
| ATOM | 4341 | O   | ASP D 171 | 115.816 | 45.090 |  5.910 | 1.00 | 48.29 | D |
| ATOM | 4342 | N   | LYS D 172 | 114.348 | 46.715 |  5.364 | 1.00 | 48.92 | D |
| ATOM | 4343 | CA  | LYS D 172 | 114.883 | 47.707 |  6.299 | 1.00 | 49.86 | D |
| ATOM | 4344 | CB  | LYS D 172 | 115.502 | 48.898 |  5.552 | 1.00 | 51.58 | D |
| ATOM | 4345 | CG  | LYS D 172 | 116.667 | 48.566 |  4.637 | 1.00 | 55.86 | D |
| ATOM | 4346 | CD  | LYS D 172 | 116.203 | 47.963 |  3.316 | 1.00 | 58.23 | D |
| ATOM | 4347 | CE  | LYS D 172 | 115.408 | 48.966 |  2.493 | 1.00 | 59.62 | D |
| ATOM | 4348 | NZ  | LYS D 172 | 114.946 | 48.368 |  1.211 | 1.00 | 59.53 | D |
| ATOM | 4349 | C   | LYS D 172 | 113.734 | 48.224 |  7.165 | 1.00 | 48.46 | D |
| ATOM | 4350 | O   | LYS D 172 | 112.564 | 48.026 |  6.833 | 1.00 | 48.43 | D |
| ATOM | 4351 | N   | PRO D 173 | 114.050 | 48.885 |  8.291 | 1.00 | 46.54 | D |
| ATOM | 4352 | CD  | PRO D 173 | 115.355 | 49.048 |  8.954 | 1.00 | 46.03 | D |
| ATOM | 4353 | CA  | PRO D 173 | 112.974 | 49.400 |  9.137 | 1.00 | 44.41 | D |
| ATOM | 4354 | CB  | PRO D 173 | 113.722 | 50.029 | 10.305 | 1.00 | 44.19 | D |
| ATOM | 4355 | CG  | PRO D 173 | 114.950 | 49.197 | 10.399 | 1.00 | 45.63 | D |
| ATOM | 4356 | C   | PRO D 173 | 112.180 | 50.430 |  8.348 | 1.00 | 43.26 | D |
| ATOM | 4357 | O   | PRO D 173 | 112.746 | 51.197 |  7.570 | 1.00 | 43.42 | D |
| ATOM | 4358 | N   | LEU D 174 | 110.869 | 50.434 |  8.532 | 1.00 | 41.53 | D |
| ATOM | 4359 | CA  | LEU D 174 | 110.023 | 51.381 |  7.829 | 1.00 | 39.96 | D |
| ATOM | 4360 | CB  | LEU D 174 | 108.675 | 50.730 |  7.523 | 1.00 | 40.30 | D |
| ATOM | 4361 | CG  | LEU D 174 | 107.900 | 51.223 |  6.303 | 1.00 | 40.55 | D |

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| ATOM | 4362 | CD1 | LEU | D | 174 | 106.637 | 50.397 | 6.151 | 1.00 | 42.25 | D |
|------|------|-----|-----|---|-----|---------|--------|-------|------|-------|---|
| ATOM | 4363 | CD2 | LEU | D | 174 | 107.568 | 52.698 | 6.448 | 1.00 | 42.67 | D |
| ATOM | 4364 | C | LEU | D | 174 | 109.845 | 52.586 | 8.753 | 1.00 | 39.80 | D |
| ATOM | 4365 | O | LEU | D | 174 | 109.645 | 52.420 | 9.955 | 1.00 | 39.99 | D |
| ATOM | 4366 | N | LEU | D | 175 | 109.947 | 53.792 | 8.200 | 1.00 | 38.49 | D |
| ATOM | 4367 | CA | LEU | D | 175 | 109.787 | 55.016 | 8.983 | 1.00 | 38.04 | D |
| ATOM | 4368 | CB | LEU | D | 175 | 111.095 | 55.812 | 9.045 | 1.00 | 38.62 | D |
| ATOM | 4369 | CG | LEU | D | 175 | 112.127 | 55.442 | 10.113 | 1.00 | 38.70 | D |
| ATOM | 4370 | CD1 | LEU | D | 175 | 111.518 | 55.648 | 11.489 | 1.00 | 39.24 | D |
| ATOM | 4371 | CD2 | LEU | D | 175 | 112.577 | 54.001 | 9.936 | 1.00 | 40.07 | D |
| ATOM | 4372 | C | LEU | D | 175 | 108.712 | 55.892 | 8.372 | 1.00 | 37.31 | D |
| ATOM | 4373 | O | LEU | D | 175 | 108.885 | 56.432 | 7.282 | 1.00 | 38.54 | D |
| ATOM | 4374 | N | LYS | D | 176 | 107.599 | 56.033 | 9.076 | 1.00 | 35.14 | D |
| ATOM | 4375 | CA | LYS | D | 176 | 106.511 | 56.850 | 8.577 | 1.00 | 34.26 | D |
| ATOM | 4376 | CB | LYS | D | 176 | 105.175 | 56.124 | 8.768 | 1.00 | 33.88 | D |
| ATOM | 4377 | CG | LYS | D | 176 | 104.204 | 56.325 | 7.620 | 1.00 | 36.72 | D |
| ATOM | 4378 | CD | LYS | D | 176 | 104.829 | 55.887 | 6.295 | 1.00 | 37.68 | D |
| ATOM | 4379 | CE | LYS | D | 176 | 103.820 | 55.913 | 5.155 | 1.00 | 39.32 | D |
| ATOM | 4380 | NZ | LYS | D | 176 | 103.195 | 57.254 | 4.974 | 1.00 | 40.75 | D |
| ATOM | 4381 | C | LYS | D | 176 | 106.523 | 58.166 | 9.335 | 1.00 | 32.22 | D |
| ATOM | 4382 | O | LYS | D | 176 | 106.272 | 58.204 | 10.537 | 1.00 | 32.35 | D |
| ATOM | 4383 | N | HIS | D | 177 | 106.825 | 59.243 | 8.625 | 1.00 | 29.85 | D |
| ATOM | 4384 | CA | HIS | D | 177 | 106.897 | 60.563 | 9.229 | 1.00 | 29.87 | D |
| ATOM | 4385 | CB | HIS | D | 177 | 107.836 | 61.456 | 8.411 | 1.00 | 30.84 | D |
| ATOM | 4386 | CG | HIS | D | 177 | 108.014 | 62.830 | 8.979 | 1.00 | 31.41 | D |
| ATOM | 4387 | CD2 | HIS | D | 177 | 107.607 | 64.042 | 8.529 | 1.00 | 32.01 | D |
| ATOM | 4388 | ND1 | HIS | D | 177 | 108.695 | 63.067 | 10.155 | 1.00 | 32.16 | D |
| ATOM | 4389 | CE1 | HIS | D | 177 | 108.704 | 64.365 | 10.402 | 1.00 | 30.49 | D |
| ATOM | 4390 | NE2 | HIS | D | 177 | 108.051 | 64.979 | 9.431 | 1.00 | 31.08 | D |
| ATOM | 4391 | C | HIS | D | 177 | 105.532 | 61.228 | 9.332 | 1.00 | 29.28 | D |
| ATOM | 4392 | O | HIS | D | 177 | 104.709 | 61.121 | 8.429 | 1.00 | 27.97 | D |
| ATOM | 4393 | N | TRP | D | 178 | 105.295 | 61.922 | 10.439 | 1.00 | 29.05 | D |
| ATOM | 4394 | CA | TRP | D | 178 | 104.031 | 62.617 | 10.619 | 1.00 | 29.38 | D |
| ATOM | 4395 | CB | TRP | D | 178 | 103.518 | 62.464 | 12.048 | 1.00 | 26.73 | D |
| ATOM | 4396 | CG | TRP | D | 178 | 102.205 | 63.165 | 12.243 | 1.00 | 27.32 | D |
| ATOM | 4397 | CD2 | TRP | D | 178 | 101.939 | 64.262 | 13.122 | 1.00 | 24.87 | D |
| ATOM | 4398 | CE2 | TRP | D | 178 | 100.580 | 64.608 | 12.959 | 1.00 | 26.97 | D |
| ATOM | 4399 | CE3 | TRP | D | 178 | 102.714 | 64.986 | 14.033 | 1.00 | 26.15 | D |
| ATOM | 4400 | CD1 | TRP | D | 178 | 101.028 | 62.898 | 11.599 | 1.00 | 26.41 | D |
| ATOM | 4401 | NE1 | TRP | D | 178 | 100.050 | 63.759 | 12.023 | 1.00 | 25.31 | D |
| ATOM | 4402 | CZ2 | TRP | D | 178 | 99.980 | 65.649 | 13.675 | 1.00 | 25.60 | D |
| ATOM | 4403 | CZ3 | TRP | D | 178 | 102.118 | 66.021 | 14.746 | 1.00 | 27.98 | D |
| ATOM | 4404 | CH2 | TRP | D | 178 | 100.763 | 66.340 | 14.562 | 1.00 | 27.02 | D |
| ATOM | 4405 | C | TRP | D | 178 | 104.185 | 64.100 | 10.294 | 1.00 | 30.33 | D |
| ATOM | 4406 | O | TRP | D | 178 | 104.756 | 64.824 | 11.143 | 1.00 | 29.85 | D |
| ATOM | 4407 | OXT | TRP | D | 178 | 103.745 | 64.512 | 9.193 | 1.00 | 32.23 | D |
| ATOM | 4408 | CB | SER | E | 3 | 113.641 | 35.776 | 8.019 | 1.00 | 59.19 | E |
| ATOM | 4409 | OG | SER | E | 3 | 112.349 | 35.748 | 8.608 | 1.00 | 59.65 | E |
| ATOM | 4410 | C | SER | E | 3 | 114.352 | 33.977 | 9.601 | 1.00 | 57.92 | E |
| ATOM | 4411 | O | SER | E | 3 | 114.571 | 32.945 | 8.970 | 1.00 | 57.45 | E |
| ATOM | 4412 | N | SER | E | 3 | 116.055 | 35.305 | 8.352 | 1.00 | 59.31 | E |
| ATOM | 4413 | CA | SER | E | 3 | 114.719 | 35.342 | 9.020 | 1.00 | 58.85 | E |
| ATOM | 4414 | N | PRO | E | 4 | 113.799 | 33.958 | 10.824 | 1.00 | 56.65 | E |
| ATOM | 4415 | CD | PRO | E | 4 | 113.679 | 35.092 | 11.759 | 1.00 | 56.20 | E |
| ATOM | 4416 | CA | PRO | E | 4 | 113.403 | 32.704 | 11.472 | 1.00 | 55.50 | E |
| ATOM | 4417 | CB | PRO | E | 4 | 113.362 | 33.086 | 12.946 | 1.00 | 56.49 | E |
| ATOM | 4418 | CG | PRO | E | 4 | 112.870 | 34.493 | 12.893 | 1.00 | 56.56 | E |
| ATOM | 4419 | C | PRO | E | 4 | 112.046 | 32.217 | 10.957 | 1.00 | 53.68 | E |
| ATOM | 4420 | O | PRO | E | 4 | 111.168 | 33.024 | 10.648 | 1.00 | 54.06 | E |
| ATOM | 4421 | N | GLU | E | 5 | 111.875 | 30.903 | 10.855 | 1.00 | 51.52 | E |
| ATOM | 4422 | CA | GLU | E | 5 | 110.610 | 30.360 | 10.373 | 1.00 | 49.69 | E |
| ATOM | 4423 | CB | GLU | E | 5 | 110.831 | 29.007 | 9.676 | 1.00 | 53.42 | E |
| ATOM | 4424 | CG | GLU | E | 5 | 111.305 | 27.867 | 10.561 | 1.00 | 57.99 | E |
| ATOM | 4425 | CD | GLU | E | 5 | 111.671 | 26.626 | 9.758 | 1.00 | 60.86 | E |
| ATOM | 4426 | OE1 | GLU | E | 5 | 110.857 | 26.196 | 8.908 | 1.00 | 62.41 | E |
| ATOM | 4427 | OE2 | GLU | E | 5 | 112.772 | 26.077 | 9.979 | 1.00 | 63.42 | E |
| ATOM | 4428 | C | GLU | E | 5 | 109.619 | 30.231 | 11.525 | 1.00 | 45.48 | E |
| ATOM | 4429 | O | GLU | E | 5 | 109.919 | 29.644 | 12.564 | 1.00 | 46.07 | E |
| ATOM | 4430 | N | ASP | E | 6 | 108.436 | 30.800 | 11.337 | 1.00 | 40.87 | E |
| ATOM | 4431 | CA | ASP | E | 6 | 107.403 | 30.782 | 12.363 | 1.00 | 36.20 | E |
| ATOM | 4432 | CB | ASP | E | 6 | 106.911 | 32.214 | 12.617 | 1.00 | 35.53 | E |
| ATOM | 4433 | CG | ASP | E | 6 | 105.995 | 32.323 | 13.827 | 1.00 | 33.60 | E |
| ATOM | 4434 | OD1 | ASP | E | 6 | 105.185 | 33.268 | 13.864 | 1.00 | 34.88 | E |
| ATOM | 4435 | OD2 | ASP | E | 6 | 106.089 | 31.487 | 14.748 | 1.00 | 33.84 | E |

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| ATOM | 4436 | C   | ASP | E | 6  | 106.229 | 29.915 | 11.938 | 1.00 | 33.07 | E |
|------|------|-----|-----|---|----|---------|--------|--------|------|-------|---|
| ATOM | 4437 | O   | ASP | E | 6  | 105.882 | 29.867 | 10.762 | 1.00 | 32.95 | E |
| ATOM | 4438 | N   | PHE | E | 7  | 105.632 | 29.228 | 12.906 | 1.00 | 31.08 | E |
| ATOM | 4439 | CA  | PHE | E | 7  | 104.466 | 28.380 | 12.669 | 1.00 | 29.18 | E |
| ATOM | 4440 | CB  | PHE | E | 7  | 104.760 | 26.950 | 13.116 | 1.00 | 31.11 | E |
| ATOM | 4441 | CG  | PHE | E | 7  | 105.833 | 26.278 | 12.305 | 1.00 | 31.97 | E |
| ATOM | 4442 | CD1 | PHE | E | 7  | 105.544 | 25.745 | 11.053 | 1.00 | 31.67 | E |
| ATOM | 4443 | CD2 | PHE | E | 7  | 107.141 | 26.200 | 12.782 | 1.00 | 32.49 | E |
| ATOM | 4444 | CE1 | PHE | E | 7  | 106.546 | 25.141 | 10.282 | 1.00 | 33.41 | E |
| ATOM | 4445 | CE2 | PHE | E | 7  | 108.148 | 25.602 | 12.023 | 1.00 | 32.29 | E |
| ATOM | 4446 | CZ  | PHE | E | 7  | 107.850 | 25.071 | 10.770 | 1.00 | 31.62 | E |
| ATOM | 4447 | C   | PHE | E | 7  | 103.345 | 28.994 | 13.504 | 1.00 | 27.19 | E |
| ATOM | 4448 | O   | PHE | E | 7  | 103.483 | 29.151 | 14.715 | 1.00 | 25.77 | E |
| ATOM | 4449 | N   | VAL | E | 8  | 102.238 | 29.340 | 12.855 | 1.00 | 25.52 | E |
| ATOM | 4450 | CA  | VAL | E | 8  | 101.127 | 29.998 | 13.538 | 1.00 | 23.97 | E |
| ATOM | 4451 | CB  | VAL | E | 8  | 100.903 | 31.411 | 12.949 | 1.00 | 22.51 | E |
| ATOM | 4452 | CG1 | VAL | E | 8  | 99.789  | 32.130 | 13.703 | 1.00 | 20.58 | E |
| ATOM | 4453 | CG2 | VAL | E | 8  | 102.205 | 32.211 | 13.002 | 1.00 | 22.51 | E |
| ATOM | 4454 | C   | VAL | E | 8  | 99.785  | 29.275 | 13.510 | 1.00 | 24.21 | E |
| ATOM | 4455 | O   | VAL | E | 8  | 99.369  | 28.736 | 12.485 | 1.00 | 25.26 | E |
| ATOM | 4456 | N   | TYR | E | 9  | 99.096  | 29.288 | 14.643 | 1.00 | 23.98 | E |
| ATOM | 4457 | CA  | TYR | E | 9  | 97.786  | 28.663 | 14.724 | 1.00 | 23.53 | E |
| ATOM | 4458 | CB  | TYR | E | 9  | 97.796  | 27.505 | 15.718 | 1.00 | 24.07 | E |
| ATOM | 4459 | CG  | TYR | E | 9  | 96.562  | 26.640 | 15.627 | 1.00 | 25.27 | E |
| ATOM | 4460 | CD1 | TYR | E | 9  | 96.570  | 25.460 | 14.889 | 1.00 | 27.68 | E |
| ATOM | 4461 | CE1 | TYR | E | 9  | 95.435  | 24.658 | 14.801 | 1.00 | 27.67 | E |
| ATOM | 4462 | CD2 | TYR | E | 9  | 95.384  | 27.002 | 16.272 | 1.00 | 24.82 | E |
| ATOM | 4463 | CE2 | TYR | E | 9  | 94.245  | 26.211 | 16.191 | 1.00 | 25.29 | E |
| ATOM | 4464 | CZ  | TYR | E | 9  | 94.277  | 25.040 | 15.458 | 1.00 | 26.82 | E |
| ATOM | 4465 | OH  | TYR | E | 9  | 93.163  | 24.240 | 15.403 | 1.00 | 27.65 | E |
| ATOM | 4466 | C   | TYR | E | 9  | 96.775  | 29.707 | 15.179 | 1.00 | 23.14 | E |
| ATOM | 4467 | O   | TYR | E | 9  | 97.037  | 30.476 | 16.106 | 1.00 | 23.66 | E |
| ATOM | 4468 | N   | GLN | E | 10 | 95.622  | 29.739 | 14.523 | 1.00 | 21.64 | E |
| ATOM | 4469 | CA  | GLN | E | 10 | 94.582  | 30.686 | 14.892 | 1.00 | 21.14 | E |
| ATOM | 4470 | CB  | GLN | E | 10 | 94.438  | 31.793 | 13.843 | 1.00 | 20.35 | E |
| ATOM | 4471 | CG  | GLN | E | 10 | 95.677  | 32.598 | 13.529 | 1.00 | 19.58 | E |
| ATOM | 4472 | CD  | GLN | E | 10 | 95.410  | 33.655 | 12.461 | 1.00 | 18.44 | E |
| ATOM | 4473 | OE1 | GLN | E | 10 | 94.498  | 34.474 | 12.593 | 1.00 | 19.00 | E |
| ATOM | 4474 | NE2 | GLN | E | 10 | 96.206  | 33.640 | 11.400 | 1.00 | 18.89 | E |
| ATOM | 4475 | C   | GLN | E | 10 | 93.232  | 29.997 | 15.006 | 1.00 | 19.74 | E |
| ATOM | 4476 | O   | GLN | E | 10 | 92.904  | 29.113 | 14.223 | 1.00 | 21.71 | E |
| ATOM | 4477 | N   | PHE | E | 11 | 92.450  | 30.408 | 15.991 | 1.00 | 19.13 | E |
| ATOM | 4478 | CA  | PHE | E | 11 | 91.108  | 29.887 | 16.145 | 1.00 | 16.86 | E |
| ATOM | 4479 | CB  | PHE | E | 11 | 90.981  | 28.881 | 17.271 | 1.00 | 16.74 | E |
| ATOM | 4480 | CG  | PHE | E | 11 | 89.562  | 28.466 | 17.517 | 1.00 | 18.71 | E |
| ATOM | 4481 | CD1 | PHE | E | 11 | 88.910  | 27.615 | 16.626 | 1.00 | 21.10 | E |
| ATOM | 4482 | CD2 | PHE | E | 11 | 88.849  | 28.985 | 18.595 | 1.00 | 18.11 | E |
| ATOM | 4483 | CE1 | PHE | E | 11 | 87.559  | 27.290 | 16.807 | 1.00 | 22.40 | E |
| ATOM | 4484 | CE2 | PHE | E | 11 | 87.499  | 28.671 | 18.789 | 1.00 | 15.75 | E |
| ATOM | 4485 | CZ  | PHE | E | 11 | 86.854  | 27.826 | 17.898 | 1.00 | 21.25 | E |
| ATOM | 4486 | C   | PHE | E | 11 | 90.218  | 31.069 | 16.451 | 1.00 | 17.10 | E |
| ATOM | 4487 | O   | PHE | E | 11 | 90.461  | 31.819 | 17.406 | 1.00 | 13.97 | E |
| ATOM | 4488 | N   | LYS | E | 12 | 89.197  | 31.241 | 15.622 | 1.00 | 16.07 | E |
| ATOM | 4489 | CA  | LYS | E | 12 | 88.266  | 32.338 | 15.789 | 1.00 | 16.96 | E |
| ATOM | 4490 | CB  | LYS | E | 12 | 88.308  | 33.246 | 14.564 | 1.00 | 17.05 | E |
| ATOM | 4491 | CG  | LYS | E | 12 | 89.703  | 33.748 | 14.200 | 1.00 | 17.57 | E |
| ATOM | 4492 | CD  | LYS | E | 12 | 89.663  | 34.535 | 12.888 | 1.00 | 18.92 | E |
| ATOM | 4493 | CE  | LYS | E | 12 | 91.018  | 35.136 | 12.532 | 1.00 | 17.07 | E |
| ATOM | 4494 | NZ  | LYS | E | 12 | 90.920  | 36.063 | 11.362 | 1.00 | 14.26 | E |
| ATOM | 4495 | C   | LYS | E | 12 | 86.856  | 31.803 | 15.987 | 1.00 | 17.87 | E |
| ATOM | 4496 | O   | LYS | E | 12 | 86.354  | 31.039 | 15.165 | 1.00 | 16.82 | E |
| ATOM | 4497 | N   | GLY | E | 13 | 86.235  | 32.195 | 17.098 | 1.00 | 18.19 | E |
| ATOM | 4498 | CA  | GLY | E | 13 | 84.875  | 31.776 | 17.391 | 1.00 | 19.62 | E |
| ATOM | 4499 | C   | GLY | E | 13 | 83.991  | 32.939 | 17.010 | 1.00 | 19.93 | E |
| ATOM | 4500 | O   | GLY | E | 13 | 83.539  | 33.695 | 17.868 | 1.00 | 21.65 | E |
| ATOM | 4501 | N   | MET | E | 14 | 83.728  | 33.070 | 15.715 | 1.00 | 19.89 | E |
| ATOM | 4502 | CA  | MET | E | 14 | 82.947  | 34.184 | 15.197 | 1.00 | 20.54 | E |
| ATOM | 4503 | CB  | MET | E | 14 | 83.430  | 34.490 | 13.785 | 1.00 | 21.02 | E |
| ATOM | 4504 | CG  | MET | E | 14 | 84.937  | 34.657 | 13.751 | 1.00 | 23.04 | E |
| ATOM | 4505 | SD  | MET | E | 14 | 85.587  | 35.218 | 12.190 | 1.00 | 25.32 | E |
| ATOM | 4506 | CE  | MET | E | 14 | 85.218  | 36.938 | 12.284 | 1.00 | 20.32 | E |
| ATOM | 4507 | C   | MET | E | 14 | 81.429  | 34.078 | 15.219 | 1.00 | 20.83 | E |
| ATOM | 4508 | O   | MET | E | 14 | 80.859  | 32.999 | 15.101 | 1.00 | 20.77 | E |
| ATOM | 4509 | N   | CYS | E | 15 | 80.789  | 35.232 | 15.377 | 1.00 | 20.66 | E |

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| ATOM | 4510 | CA | CYS | E | 15 | 79.332 | 35.336 | 15.418 | 1.00 | 22.09 | E |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 4511 | C | CYS | E | 15 | 78.882 | 36.495 | 14.524 | 1.00 | 21.39 | E |
| ATOM | 4512 | O | CYS | E | 15 | 79.393 | 37.614 | 14.644 | 1.00 | 19.38 | E |
| ATOM | 4513 | CB | CYS | E | 15 | 78.841 | 35.616 | 16.848 | 1.00 | 22.10 | E |
| ATOM | 4514 | SG | CYS | E | 15 | 78.970 | 34.281 | 18.094 | 1.00 | 26.75 | E |
| ATOM | 4515 | N | TYR | E | 16 | 77.931 | 36.229 | 13.633 | 1.00 | 20.94 | E |
| ATOM | 4516 | CA | TYR | E | 16 | 77.408 | 37.270 | 12.752 | 1.00 | 21.23 | E |
| ATOM | 4517 | CB | TYR | E | 16 | 77.548 | 36.858 | 11.287 | 1.00 | 18.37 | E |
| ATOM | 4518 | CG | TYR | E | 16 | 78.972 | 36.574 | 10.876 | 1.00 | 19.23 | E |
| ATOM | 4519 | CD1 | TYR | E | 16 | 79.576 | 35.354 | 11.178 | 1.00 | 18.71 | E |
| ATOM | 4520 | CE1 | TYR | E | 16 | 80.875 | 35.084 | 10.789 | 1.00 | 18.69 | E |
| ATOM | 4521 | CD2 | TYR | E | 16 | 79.715 | 37.524 | 10.178 | 1.00 | 20.25 | E |
| ATOM | 4522 | CE2 | TYR | E | 16 | 81.022 | 37.270 | 9.785 | 1.00 | 17.18 | E |
| ATOM | 4523 | CZ | TYR | E | 16 | 81.595 | 36.047 | 10.088 | 1.00 | 21.03 | E |
| ATOM | 4524 | OH | TYR | E | 16 | 82.872 | 35.775 | 9.662 | 1.00 | 22.99 | E |
| ATOM | 4525 | C | TYR | E | 16 | 75.938 | 37.543 | 13.085 | 1.00 | 22.17 | E |
| ATOM | 4526 | O | TYR | E | 16 | 75.132 | 36.612 | 13.199 | 1.00 | 21.71 | E |
| ATOM | 4527 | N | PHE | E | 17 | 75.607 | 38.825 | 13.247 | 1.00 | 23.05 | E |
| ATOM | 4528 | CA | PHE | E | 17 | 74.254 | 39.263 | 13.591 | 1.00 | 23.67 | E |
| ATOM | 4529 | CB | PHE | E | 17 | 74.261 | 39.988 | 14.942 | 1.00 | 22.49 | E |
| ATOM | 4530 | CG | PHE | E | 17 | 74.813 | 39.172 | 16.084 | 1.00 | 25.10 | E |
| ATOM | 4531 | CD1 | PHE | E | 17 | 74.007 | 38.270 | 16.772 | 1.00 | 24.22 | E |
| ATOM | 4532 | CD2 | PHE | E | 17 | 76.140 | 39.318 | 16.482 | 1.00 | 24.67 | E |
| ATOM | 4533 | CE1 | PHE | E | 17 | 74.516 | 37.526 | 17.844 | 1.00 | 24.68 | E |
| ATOM | 4534 | CE2 | PHE | E | 17 | 76.656 | 38.579 | 17.548 | 1.00 | 24.45 | E |
| ATOM | 4535 | CZ | PHE | E | 17 | 75.843 | 37.684 | 18.228 | 1.00 | 24.13 | E |
| ATOM | 4536 | C | PHE | E | 17 | 73.673 | 40.223 | 12.549 | 1.00 | 25.10 | E |
| ATOM | 4537 | O | PHE | E | 17 | 74.390 | 41.034 | 11.971 | 1.00 | 24.65 | E |
| ATOM | 4538 | N | THR | E | 18 | 72.365 | 40.122 | 12.333 | 1.00 | 27.15 | E |
| ATOM | 4539 | CA | THR | E | 18 | 71.638 | 40.983 | 11.405 | 1.00 | 29.69 | E |
| ATOM | 4540 | CB | THR | E | 18 | 71.609 | 40.397 | 9.978 | 1.00 | 29.46 | E |
| ATOM | 4541 | OG1 | THR | E | 18 | 72.949 | 40.252 | 9.500 | 1.00 | 32.31 | E |
| ATOM | 4542 | CG2 | THR | E | 18 | 70.863 | 41.321 | 9.032 | 1.00 | 28.09 | E |
| ATOM | 4543 | C | THR | E | 18 | 70.217 | 41.080 | 11.950 | 1.00 | 31.56 | E |
| ATOM | 4544 | O | THR | E | 18 | 69.638 | 40.071 | 12.355 | 1.00 | 32.09 | E |
| ATOM | 4545 | N | ASN | E | 19 | 69.661 | 42.290 | 11.969 | 1.00 | 33.38 | E |
| ATOM | 4546 | CA | ASN | E | 19 | 68.316 | 42.495 | 12.497 | 1.00 | 35.02 | E |
| ATOM | 4547 | CB | ASN | E | 19 | 67.279 | 41.755 | 11.647 | 1.00 | 37.99 | E |
| ATOM | 4548 | CG | ASN | E | 19 | 66.779 | 42.587 | 10.489 | 1.00 | 42.21 | E |
| ATOM | 4549 | OD1 | ASN | E | 19 | 66.271 | 43.695 | 10.687 | 1.00 | 47.70 | E |
| ATOM | 4550 | ND2 | ASN | E | 19 | 66.910 | 42.063 | 9.273 | 1.00 | 43.13 | E |
| ATOM | 4551 | C | ASN | E | 19 | 68.264 | 41.977 | 13.924 | 1.00 | 34.10 | E |
| ATOM | 4552 | O | ASN | E | 19 | 67.487 | 41.077 | 14.233 | 1.00 | 34.27 | E |
| ATOM | 4553 | N | GLY | E | 20 | 69.088 | 42.553 | 14.795 | 1.00 | 33.50 | E |
| ATOM | 4554 | CA | GLY | E | 20 | 69.120 | 42.106 | 16.175 | 1.00 | 33.61 | E |
| ATOM | 4555 | C | GLY | E | 20 | 69.575 | 40.663 | 16.175 | 1.00 | 33.98 | E |
| ATOM | 4556 | O | GLY | E | 20 | 70.580 | 40.343 | 15.541 | 1.00 | 34.56 | E |
| ATOM | 4557 | N | THR | E | 21 | 68.847 | 39.789 | 16.866 | 1.00 | 34.08 | E |
| ATOM | 4558 | CA | THR | E | 21 | 69.198 | 38.372 | 16.897 | 1.00 | 35.71 | E |
| ATOM | 4559 | CB | THR | E | 21 | 69.193 | 37.809 | 18.335 | 1.00 | 37.69 | E |
| ATOM | 4560 | OG1 | THR | E | 21 | 67.907 | 38.026 | 18.930 | 1.00 | 39.78 | E |
| ATOM | 4561 | CG2 | THR | E | 21 | 70.268 | 38.480 | 19.174 | 1.00 | 38.05 | E |
| ATOM | 4562 | C | THR | E | 21 | 68.251 | 37.517 | 16.050 | 1.00 | 35.19 | E |
| ATOM | 4563 | O | THR | E | 21 | 68.092 | 36.324 | 16.303 | 1.00 | 36.08 | E |
| ATOM | 4564 | N | GLU | E | 22 | 67.619 | 38.129 | 15.052 | 1.00 | 34.15 | E |
| ATOM | 4565 | CA | GLU | E | 22 | 66.705 | 37.405 | 14.176 | 1.00 | 34.08 | E |
| ATOM | 4566 | CB | GLU | E | 22 | 65.868 | 38.388 | 13.354 | 1.00 | 33.12 | E |
| ATOM | 4567 | CG | GLU | E | 22 | 64.781 | 39.073 | 14.164 | 1.00 | 33.66 | E |
| ATOM | 4568 | CD | GLU | E | 22 | 64.173 | 40.266 | 13.451 | 1.00 | 35.85 | E |
| ATOM | 4569 | OE1 | GLU | E | 22 | 63.865 | 40.151 | 12.244 | 1.00 | 35.10 | E |
| ATOM | 4570 | OE2 | GLU | E | 22 | 63.995 | 41.317 | 14.105 | 1.00 | 38.34 | E |
| ATOM | 4571 | C | GLU | E | 22 | 67.523 | 36.503 | 13.265 | 1.00 | 33.80 | E |
| ATOM | 4572 | O | GLU | E | 22 | 67.205 | 35.329 | 13.092 | 1.00 | 34.50 | E |
| ATOM | 4573 | N | ARG | E | 23 | 68.574 | 37.065 | 12.678 | 1.00 | 33.59 | E |
| ATOM | 4574 | CA | ARG | E | 23 | 69.467 | 36.298 | 11.818 | 1.00 | 33.75 | E |
| ATOM | 4575 | CB | ARG | E | 23 | 69.703 | 36.996 | 10.470 | 1.00 | 36.33 | E |
| ATOM | 4576 | CG | ARG | E | 23 | 68.599 | 36.815 | 9.434 | 1.00 | 42.06 | E |
| ATOM | 4577 | CD | ARG | E | 23 | 67.342 | 37.577 | 9.813 | 1.00 | 47.83 | E |
| ATOM | 4578 | NE | ARG | E | 23 | 66.408 | 37.696 | 8.695 | 1.00 | 51.02 | E |
| ATOM | 4579 | CZ | ARG | E | 23 | 65.349 | 38.502 | 8.690 | 1.00 | 52.66 | E |
| ATOM | 4580 | NH1 | ARG | E | 23 | 65.087 | 39.263 | 9.747 | 1.00 | 50.82 | E |
| ATOM | 4581 | NH2 | ARG | E | 23 | 64.555 | 38.555 | 7.626 | 1.00 | 53.53 | E |
| ATOM | 4582 | C | ARG | E | 23 | 70.788 | 36.177 | 12.560 | 1.00 | 30.98 | E |
| ATOM | 4583 | O | ARG | E | 23 | 71.465 | 37.172 | 12.827 | 1.00 | 30.90 | E |

| ATOM | 4584 | N | VAL | E | 24 | 71.149 | 34.955 | 12.909 | 1.00 | 28.33 | E |
| ATOM | 4585 | CA | VAL | E | 24 | 72.394 | 34.735 | 13.621 | 1.00 | 25.06 | E |
| ATOM | 4586 | CB | VAL | E | 24 | 72.148 | 34.500 | 15.129 | 1.00 | 22.98 | E |
| ATOM | 4587 | CG1 | VAL | E | 24 | 73.456 | 34.106 | 15.817 | 1.00 | 21.05 | E |
| ATOM | 4588 | CG2 | VAL | E | 24 | 71.582 | 35.762 | 15.763 | 1.00 | 21.04 | E |
| ATOM | 4589 | C | VAL | E | 24 | 73.144 | 33.550 | 13.049 | 1.00 | 23.08 | E |
| ATOM | 4590 | O | VAL | E | 24 | 72.600 | 32.458 | 12.914 | 1.00 | 24.17 | E |
| ATOM | 4591 | N | ARG | E | 25 | 74.398 | 33.778 | 12.694 | 1.00 | 23.02 | E |
| ATOM | 4592 | CA | ARG | E | 25 | 75.223 | 32.718 | 12.156 | 1.00 | 23.30 | E |
| ATOM | 4593 | CB | ARG | E | 25 | 75.511 | 32.930 | 10.659 | 1.00 | 24.06 | E |
| ATOM | 4594 | CG | ARG | E | 25 | 76.653 | 32.044 | 10.176 | 1.00 | 25.99 | E |
| ATOM | 4595 | CD | ARG | E | 25 | 76.470 | 31.478 | 8.774 | 1.00 | 28.29 | E |
| ATOM | 4596 | NE | ARG | E | 25 | 76.468 | 32.502 | 7.743 | 1.00 | 29.69 | E |
| ATOM | 4597 | CZ | ARG | E | 25 | 76.786 | 32.287 | 6.466 | 1.00 | 29.57 | E |
| ATOM | 4598 | NH1 | ARG | E | 25 | 77.145 | 31.075 | 6.047 | 1.00 | 27.28 | E |
| ATOM | 4599 | NH2 | ARG | E | 25 | 76.733 | 33.293 | 5.604 | 1.00 | 26.98 | E |
| ATOM | 4600 | C | ARG | E | 25 | 76.535 | 32.631 | 12.916 | 1.00 | 22.65 | E |
| ATOM | 4601 | O | ARG | E | 25 | 77.261 | 33.620 | 13.041 | 1.00 | 22.47 | E |
| ATOM | 4602 | N | LEU | E | 26 | 76.828 | 31.444 | 13.433 | 1.00 | 21.04 | E |
| ATOM | 4603 | CA | LEU | E | 26 | 78.069 | 31.227 | 14.152 | 1.00 | 21.94 | E |
| ATOM | 4604 | CB | LEU | E | 26 | 77.834 | 30.338 | 15.383 | 1.00 | 21.37 | E |
| ATOM | 4605 | CG | LEU | E | 26 | 79.054 | 29.778 | 16.128 | 1.00 | 22.89 | E |
| ATOM | 4606 | CD1 | LEU | E | 26 | 78.723 | 29.567 | 17.602 | 1.00 | 25.16 | E |
| ATOM | 4607 | CD2 | LEU | E | 26 | 79.483 | 28.466 | 15.493 | 1.00 | 23.51 | E |
| ATOM | 4608 | C | LEU | E | 26 | 79.032 | 30.552 | 13.193 | 1.00 | 21.17 | E |
| ATOM | 4609 | O | LEU | E | 26 | 78.637 | 29.674 | 12.432 | 1.00 | 21.77 | E |
| ATOM | 4610 | N | VAL | E | 27 | 80.285 | 30.983 | 13.201 | 1.00 | 19.92 | E |
| ATOM | 4611 | CA | VAL | E | 27 | 81.278 | 30.358 | 12.345 | 1.00 | 21.31 | E |
| ATOM | 4612 | CB | VAL | E | 27 | 81.530 | 31.166 | 11.039 | 1.00 | 20.44 | E |
| ATOM | 4613 | CG1 | VAL | E | 27 | 82.524 | 30.420 | 10.156 | 1.00 | 21.63 | E |
| ATOM | 4614 | CG2 | VAL | E | 27 | 80.221 | 31.366 | 10.275 | 1.00 | 20.48 | E |
| ATOM | 4615 | C | VAL | E | 27 | 82.581 | 30.231 | 13.112 | 1.00 | 21.74 | E |
| ATOM | 4616 | O | VAL | E | 27 | 83.189 | 31.228 | 13.487 | 1.00 | 24.11 | E |
| ATOM | 4617 | N | SER | E | 28 | 82.994 | 29.001 | 13.383 | 1.00 | 20.88 | E |
| ATOM | 4618 | CA | SER | E | 28 | 84.249 | 28.799 | 14.084 | 1.00 | 21.53 | E |
| ATOM | 4619 | CB | SER | E | 28 | 84.113 | 27.702 | 15.152 | 1.00 | 20.62 | E |
| ATOM | 4620 | OG | SER | E | 28 | 83.693 | 26.475 | 14.598 | 1.00 | 29.22 | E |
| ATOM | 4621 | C | SER | E | 28 | 85.274 | 28.433 | 13.006 | 1.00 | 21.41 | E |
| ATOM | 4622 | O | SER | E | 28 | 84.992 | 27.631 | 12.105 | 1.00 | 19.11 | E |
| ATOM | 4623 | N | ARG | E | 29 | 86.450 | 29.051 | 13.090 | 1.00 | 18.23 | E |
| ATOM | 4624 | CA | ARG | E | 29 | 87.496 | 28.838 | 12.105 | 1.00 | 18.45 | E |
| ATOM | 4625 | CB | ARG | E | 29 | 87.701 | 30.124 | 11.287 | 1.00 | 16.91 | E |
| ATOM | 4626 | CG | ARG | E | 29 | 86.433 | 30.817 | 10.810 | 1.00 | 17.70 | E |
| ATOM | 4627 | CD | ARG | E | 29 | 86.791 | 32.117 | 10.109 | 1.00 | 18.98 | E |
| ATOM | 4628 | NE | ARG | E | 29 | 85.631 | 32.902 | 9.705 | 1.00 | 20.82 | E |
| ATOM | 4629 | CZ | ARG | E | 29 | 84.939 | 32.704 | 8.586 | 1.00 | 22.76 | E |
| ATOM | 4630 | NH1 | ARG | E | 29 | 85.285 | 31.739 | 7.743 | 1.00 | 21.05 | E |
| ATOM | 4631 | NH2 | ARG | E | 29 | 83.904 | 33.482 | 8.309 | 1.00 | 20.13 | E |
| ATOM | 4632 | C | ARG | E | 29 | 88.842 | 28.435 | 12.710 | 1.00 | 18.44 | E |
| ATOM | 4633 | O | ARG | E | 29 | 89.401 | 29.171 | 13.520 | 1.00 | 19.35 | E |
| ATOM | 4634 | N | SER | E | 30 | 89.351 | 27.269 | 12.315 | 1.00 | 18.98 | E |
| ATOM | 4635 | CA | SER | E | 30 | 90.657 | 26.788 | 12.774 | 1.00 | 21.70 | E |
| ATOM | 4636 | CB | SER | E | 30 | 90.619 | 25.284 | 13.028 | 1.00 | 22.10 | E |
| ATOM | 4637 | OG | SER | E | 30 | 89.718 | 24.969 | 14.072 | 1.00 | 27.24 | E |
| ATOM | 4638 | C | SER | E | 30 | 91.637 | 27.119 | 11.639 | 1.00 | 23.03 | E |
| ATOM | 4639 | O | SER | E | 30 | 91.509 | 26.604 | 10.528 | 1.00 | 23.56 | E |
| ATOM | 4640 | N | ILE | E | 31 | 92.611 | 27.978 | 11.927 | 1.00 | 23.05 | E |
| ATOM | 4641 | CA | ILE | E | 31 | 93.560 | 28.439 | 10.923 | 1.00 | 22.24 | E |
| ATOM | 4642 | CB | ILE | E | 31 | 93.563 | 29.997 | 10.856 | 1.00 | 22.84 | E |
| ATOM | 4643 | CG2 | ILE | E | 31 | 94.163 | 30.470 | 9.545 | 1.00 | 19.19 | E |
| ATOM | 4644 | CG1 | ILE | E | 31 | 92.143 | 30.546 | 11.043 | 1.00 | 24.76 | E |
| ATOM | 4645 | CD1 | ILE | E | 31 | 91.144 | 30.032 | 10.047 | 1.00 | 29.25 | E |
| ATOM | 4646 | C | ILE | E | 31 | 95.013 | 28.014 | 11.134 | 1.00 | 24.53 | E |
| ATOM | 4647 | O | ILE | E | 31 | 95.566 | 28.187 | 12.225 | 1.00 | 22.94 | E |
| ATOM | 4648 | N | TYR | E | 32 | 95.625 | 27.468 | 10.081 | 1.00 | 24.41 | E |
| ATOM | 4649 | CA | TYR | E | 32 | 97.030 | 27.089 | 10.120 | 1.00 | 24.27 | E |
| ATOM | 4650 | CB | TYR | E | 32 | 97.277 | 25.755 | 9.417 | 1.00 | 26.61 | E |
| ATOM | 4651 | CG | TYR | E | 32 | 98.733 | 25.338 | 9.444 | 1.00 | 29.24 | E |
| ATOM | 4652 | CD1 | TYR | E | 32 | 99.423 | 25.231 | 10.649 | 1.00 | 30.69 | E |
| ATOM | 4653 | CE1 | TYR | E | 32 | 100.770 | 24.880 | 10.683 | 1.00 | 32.83 | E |
| ATOM | 4654 | CD2 | TYR | E | 32 | 99.426 | 25.078 | 8.267 | 1.00 | 31.46 | E |
| ATOM | 4655 | CE2 | TYR | E | 32 | 100.774 | 24.721 | 8.288 | 1.00 | 32.58 | E |
| ATOM | 4656 | CZ | TYR | E | 32 | 101.438 | 24.625 | 9.497 | 1.00 | 32.80 | E |
| ATOM | 4657 | OH | TYR | E | 32 | 102.768 | 24.280 | 9.522 | 1.00 | 33.44 | E |

| ATOM | 4658 | C    | TYR | E | 32 | 97.700  | 28.225 | 9.353  | 1.00 24.83 | E |
|------|------|------|-----|---|----|---------|--------|--------|------------|---|
| ATOM | 4659 | O    | TYR | E | 32 | 97.444  | 28.415 | 8.164  | 1.00 25.49 | E |
| ATOM | 4660 | N    | ASN | E | 33 | 98.543  | 28.985 | 10.045 | 1.00 24.28 | E |
| ATOM | 4661 | CA   | ASN | E | 33 | 99.202  | 30.146 | 9.461  | 1.00 24.25 | E |
| ATOM | 4662 | CB   | ASN | E | 33 | 100.144 | 29.740 | 8.324  | 1.00 23.93 | E |
| ATOM | 4663 | CG   | ASN | E | 33 | 101.379 | 29.014 | 8.834  | 1.00 25.26 | E |
| ATOM | 4664 | OD1  | ASN | E | 33 | 102.003 | 29.439 | 9.808  | 1.00 26.40 | E |
| ATOM | 4665 | ND2  | ASN | E | 33 | 101.737 | 27.918 | 8.181  | 1.00 25.47 | E |
| ATOM | 4666 | C    | ASN | E | 33 | 98.114  | 31.099 | 8.980  | 1.00 24.88 | E |
| ATOM | 4667 | O    | ASN | E | 33 | 97.494  | 31.780 | 9.799  | 1.00 25.88 | E |
| ATOM | 4668 | N    | ARG | E | 34 | 97.864  | 31.163 | 7.677  | 1.00 24.52 | E |
| ATOM | 4669 | CA   | ARG | E | 34 | 96.815  | 32.055 | 7.194  | 1.00 26.32 | E |
| ATOM | 4670 | CB   | ARG | E | 34 | 97.385  | 33.175 | 6.317  | 1.00 26.61 | E |
| ATOM | 4671 | CG   | ARG | E | 34 | 97.999  | 34.346 | 7.072  | 1.00 26.37 | E |
| ATOM | 4672 | CD   | ARG | E | 34 | 97.776  | 35.646 | 6.304  | 1.00 28.18 | E |
| ATOM | 4673 | NE   | ARG | E | 34 | 97.886  | 35.429 | 4.865  | 1.00 31.86 | E |
| ATOM | 4674 | CZ   | ARG | E | 34 | 97.607  | 36.332 | 3.931  | 1.00 33.42 | E |
| ATOM | 4675 | NH1  | ARG | E | 34 | 97.197  | 37.550 | 4.265  | 1.00 35.40 | E |
| ATOM | 4676 | NH2  | ARG | E | 34 | 97.722  | 36.003 | 2.653  | 1.00 35.29 | E |
| ATOM | 4677 | C    | ARG | E | 34 | 95.728  | 31.333 | 6.417  | 1.00 26.98 | E |
| ATOM | 4678 | O    | ARG | E | 34 | 94.896  | 31.968 | 5.763  | 1.00 28.88 | E |
| ATOM | 4679 | N    | GLU | E | 35 | 95.719  | 30.010 | 6.481  | 1.00 26.13 | E |
| ATOM | 4680 | CA   | GLU | E | 35 | 94.698  | 29.279 | 5.759  | 1.00 27.02 | E |
| ATOM | 4681 | CB   | GLU | E | 35 | 95.350  | 28.359 | 4.720  | 1.00 31.96 | E |
| ATOM | 4682 | CG   | GLU | E | 35 | 96.284  | 27.301 | 5.278  | 1.00 38.52 | E |
| ATOM | 4683 | CD   | GLU | E | 35 | 97.116  | 26.633 | 4.192  | 1.00 42.24 | E |
| ATOM | 4684 | OE1  | GLU | E | 35 | 98.180  | 27.187 | 3.832  | 1.00 44.86 | E |
| ATOM | 4685 | OE2  | GLU | E | 35 | 96.699  | 25.565 | 3.690  | 1.00 43.70 | E |
| ATOM | 4686 | C    | GLU | E | 35 | 93.754  | 28.498 | 6.671  | 1.00 25.31 | E |
| ATOM | 4687 | O    | GLU | E | 35 | 94.175  | 27.709 | 7.522  | 1.00 22.18 | E |
| ATOM | 4688 | N    | GLU | E | 36 | 92.464  | 28.756 | 6.498  | 1.00 24.46 | E |
| ATOM | 4689 | CA   | GLU | E | 36 | 91.438  | 28.085 | 7.272  | 1.00 24.13 | E |
| ATOM | 4690 | CB   | GLU | E | 36 | 90.085  | 28.731 | 7.001  | 1.00 24.37 | E |
| ATOM | 4691 | CG   | GLU | E | 36 | 88.975  | 28.295 | 7.928  | 1.00 25.26 | E |
| ATOM | 4692 | CD   | GLU | E | 36 | 87.669  | 28.991 | 7.604  | 1.00 26.01 | E |
| ATOM | 4693 | OE1  | GLU | E | 36 | 87.672  | 29.847 | 6.694  | 1.00 27.25 | E |
| ATOM | 4694 | OE2  | GLU | E | 36 | 86.646  | 28.689 | 8.253  | 1.00 27.12 | E |
| ATOM | 4695 | C    | GLU | E | 36 | 91.413  | 26.630 | 6.826  | 1.00 23.40 | E |
| ATOM | 4696 | O    | GLU | E | 36 | 91.252  | 26.347 | 5.645  | 1.00 23.72 | E |
| ATOM | 4697 | N    | ILE | E | 37 | 91.576  | 25.707 | 7.767  | 1.00 23.97 | E |
| ATOM | 4698 | CA   | ILE | E | 37 | 91.579  | 24.294 | 7.419  | 1.00 24.33 | E |
| ATOM | 4699 | CB   | ILE | E | 37 | 92.818  | 23.578 | 8.019  | 1.00 24.98 | E |
| ATOM | 4700 | CG2  | ILE | E | 37 | 94.096  | 24.255 | 7.532  | 1.00 24.26 | E |
| ATOM | 4701 | CG1  | ILE | E | 37 | 92.771  | 23.616 | 9.544  | 1.00 25.10 | E |
| ATOM | 4702 | CD1  | ILE | E | 37 | 93.822  | 22.742 | 10.204 | 1.00 26.49 | E |
| ATOM | 4703 | C    | ILE | E | 37 | 90.301  | 23.555 | 7.836  | 1.00 23.49 | E |
| ATOM | 4704 | O    | ILE | E | 37 | 89.871  | 22.627 | 7.162  | 1.00 23.62 | E |
| ATOM | 4705 | N    | VAL | E | 38 | 89.690  | 23.975 | 8.936  | 1.00 25.16 | E |
| ATOM | 4706 | CA   | VAL | E | 38 | 88.465  | 23.342 | 9.415  | 1.00 25.85 | E |
| ATOM | 4707 | CB   | VAL | E | 38 | 88.715  | 22.489 | 10.667 | 1.00 26.44 | E |
| ATOM | 4708 | CG1  | VAL | E | 38 | 87.516  | 21.610 | 10.932 | 1.00 27.10 | E |
| ATOM | 4709 | CG2  | VAL | E | 38 | 89.980  | 21.671 | 10.495 | 1.00 29.59 | E |
| ATOM | 4710 | C    | VAL | E | 38 | 87.481  | 24.428 | 9.792  | 1.00 24.45 | E |
| ATOM | 4711 | O    | VAL | E | 38 | 87.885  | 25.471 | 10.288 | 1.00 24.36 | E |
| ATOM | 4712 | N    | ARG | E | 39 | 86.193  | 24.168 | 9.594  | 1.00 24.90 | E |
| ATOM | 4713 | CA   | ARG | E | 39 | 85.175  | 25.161 | 9.904  | 1.00 23.66 | E |
| ATOM | 4714 | CB   | ARG | E | 39 | 84.975  | 26.055 | 8.678  | 1.00 25.55 | E |
| ATOM | 4715 | CG   | ARG | E | 39 | 83.956  | 27.174 | 8.857  | 1.00 29.11 | E |
| ATOM | 4716 | CD   | ARG | E | 39 | 83.514  | 27.755 | 7.515  | 1.00 29.37 | E |
| ATOM | 4717 | NE   | ARG | E | 39 | 84.626  | 28.289 | 6.739  | 1.00 29.70 | E |
| ATOM | 4718 | CZ   | ARG | E | 39 | 84.505  | 28.798 | 5.516  | 1.00 31.37 | E |
| ATOM | 4719 | NH1  | ARG | E | 39 | 83.314  | 28.842 | 4.930  | 1.00 33.54 | E |
| ATOM | 4720 | NH2  | ARG | E | 39 | 85.572  | 29.266 | 4.879  | 1.00 27.78 | E |
| ATOM | 4721 | C    | ARG | E | 39 | 83.813  | 24.594 | 10.328 | 1.00 23.51 | E |
| ATOM | 4722 | O    | ARG | E | 39 | 83.385  | 23.539 | 9.853  | 1.00 23.83 | E |
| ATOM | 4723 | N    | PHE | E | 40 | 83.147  | 25.295 | 11.242 | 1.00 22.04 | E |
| ATOM | 4724 | CA   | PHE | E | 40 | 81.799  | 24.918 | 11.655 | 1.00 21.92 | E |
| ATOM | 4725 | CB   | PHE | E | 40 | 81.682  | 24.551 | 13.137 | 1.00 21.36 | E |
| ATOM | 4726 | CG   | PHE | E | 40 | 80.296  | 24.088 | 13.514 | 1.00 17.04 | E |
| ATOM | 4727 | CD1  | PHE | E | 40 | 79.944  | 22.748 | 13.407 | 1.00 19.76 | E |
| ATOM | 4728 | CD2  | PHE | E | 40 | 79.315  | 25.004 | 13.875 | 1.00 16.82 | E |
| ATOM | 4729 | CE1  | PHE | E | 40 | 78.628  | 22.324 | 13.649 | 1.00 17.84 | E |
| ATOM | 4730 | CE2  | PHE | E | 40 | 78.001  | 24.594 | 14.119 | 1.00 18.10 | E |
| ATOM | 4731 | CZ   | PHE | E | 40 | 77.661  | 23.248 | 14.003 | 1.00 16.61 | E |

| ATOM | 4732 | C    | PHE | E | 40 | 80.938 | 26.148 | 11.395 | 1.00 | 21.77 | E |
|------|------|------|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 4733 | O    | PHE | E | 40 | 81.064 | 27.167 | 12.071 | 1.00 | 20.81 | E |
| ATOM | 4734 | N    | ASP | E | 41 | 80.067 | 26.033 | 10.404 | 1.00 | 21.82 | E |
| ATOM | 4735 | CA   | ASP | E | 41 | 79.181 | 27.110 | 9.995  | 1.00 | 21.76 | E |
| ATOM | 4736 | CB   | ASP | E | 41 | 79.190 | 27.182 | 8.470  | 1.00 | 22.62 | E |
| ATOM | 4737 | CG   | ASP | E | 41 | 78.492 | 28.400 | 7.929  | 1.00 | 23.09 | E |
| ATOM | 4738 | OD1  | ASP | E | 41 | 77.507 | 28.864 | 8.546  | 1.00 | 22.57 | E |
| ATOM | 4739 | OD2  | ASP | E | 41 | 78.929 | 28.881 | 6.861  | 1.00 | 25.40 | E |
| ATOM | 4740 | C    | ASP | E | 41 | 77.801 | 26.713 | 10.493 | 1.00 | 21.43 | E |
| ATOM | 4741 | O    | ASP | E | 41 | 77.277 | 25.672 | 10.085 | 1.00 | 22.83 | E |
| ATOM | 4742 | N    | SER | E | 42 | 77.210 | 27.520 | 11.369 | 1.00 | 19.04 | E |
| ATOM | 4743 | CA   | SER | E | 42 | 75.896 | 27.173 | 11.895 | 1.00 | 20.39 | E |
| ATOM | 4744 | CB   | SER | E | 42 | 75.399 | 28.220 | 12.907 | 1.00 | 19.13 | E |
| ATOM | 4745 | OG   | SER | E | 42 | 75.271 | 29.505 | 12.323 | 1.00 | 24.30 | E |
| ATOM | 4746 | C    | SER | E | 42 | 74.891 | 27.000 | 10.762 | 1.00 | 20.23 | E |
| ATOM | 4747 | O    | SER | E | 42 | 73.916 | 26.267 | 10.910 | 1.00 | 18.97 | E |
| ATOM | 4748 | N    | ASP | E | 43 | 75.145 | 27.660 | 9.631  | 1.00 | 21.77 | E |
| ATOM | 4749 | CA   | ASP | E | 43 | 74.261 | 27.556 | 8.470  | 1.00 | 24.99 | E |
| ATOM | 4750 | CB   | ASP | E | 43 | 74.561 | 28.651 | 7.439  | 1.00 | 26.10 | E |
| ATOM | 4751 | CG   | ASP | E | 43 | 73.819 | 29.947 | 7.727  | 1.00 | 28.71 | E |
| ATOM | 4752 | OD1  | ASP | E | 43 | 73.078 | 30.013 | 8.737  | 1.00 | 28.83 | E |
| ATOM | 4753 | OD2  | ASP | E | 43 | 73.976 | 30.902 | 6.939  | 1.00 | 31.35 | E |
| ATOM | 4754 | C    | ASP | E | 43 | 74.378 | 26.193 | 7.809  | 1.00 | 25.68 | E |
| ATOM | 4755 | O    | ASP | E | 43 | 73.424 | 25.727 | 7.190  | 1.00 | 28.27 | E |
| ATOM | 4756 | N    | VAL | E | 44 | 75.544 | 25.558 | 7.937  | 1.00 | 25.47 | E |
| ATOM | 4757 | CA   | VAL | E | 44 | 75.764 | 24.229 | 7.362  | 1.00 | 23.51 | E |
| ATOM | 4758 | CB   | VAL | E | 44 | 77.251 | 24.007 | 6.964  | 1.00 | 24.39 | E |
| ATOM | 4759 | CG1  | VAL | E | 44 | 77.456 | 22.579 | 6.491  | 1.00 | 19.52 | E |
| ATOM | 4760 | CG2  | VAL | E | 44 | 77.655 | 24.984 | 5.867  | 1.00 | 23.79 | E |
| ATOM | 4761 | C    | VAL | E | 44 | 75.356 | 23.154 | 8.373  | 1.00 | 23.25 | E |
| ATOM | 4762 | O    | VAL | E | 44 | 74.774 | 22.136 | 8.005  | 1.00 | 22.01 | E |
| ATOM | 4763 | N    | GLY | E | 45 | 75.683 | 23.370 | 9.644  | 1.00 | 22.52 | E |
| ATOM | 4764 | CA   | GLY | E | 45 | 75.292 | 22.411 | 10.664 | 1.00 | 21.82 | E |
| ATOM | 4765 | C    | GLY | E | 45 | 76.275 | 21.311 | 11.001 | 1.00 | 22.07 | E |
| ATOM | 4766 | O    | GLY | E | 45 | 75.982 | 20.442 | 11.818 | 1.00 | 22.49 | E |
| ATOM | 4767 | N    | GLU | E | 46 | 77.439 | 21.317 | 10.373 | 1.00 | 22.18 | E |
| ATOM | 4768 | CA   | GLU | E | 46 | 78.421 | 20.295 | 10.691 | 1.00 | 23.77 | E |
| ATOM | 4769 | CB   | GLU | E | 46 | 78.147 | 19.017 | 9.891  | 1.00 | 26.29 | E |
| ATOM | 4770 | CG   | GLU | E | 46 | 78.455 | 19.112 | 8.411  | 1.00 | 28.23 | E |
| ATOM | 4771 | CD   | GLU | E | 46 | 78.214 | 17.795 | 7.677  | 1.00 | 32.67 | E |
| ATOM | 4772 | OE1  | GLU | E | 46 | 78.575 | 17.706 | 6.482  | 1.00 | 33.19 | E |
| ATOM | 4773 | OE2  | GLU | E | 46 | 77.661 | 16.855 | 8.290  | 1.00 | 33.19 | E |
| ATOM | 4774 | C    | GLU | E | 46 | 79.807 | 20.839 | 10.383 | 1.00 | 23.15 | E |
| ATOM | 4775 | O    | GLU | E | 46 | 79.943 | 21.880 | 9.747  | 1.00 | 23.06 | E |
| ATOM | 4776 | N    | PHE | E | 47 | 80.835 | 20.153 | 10.857 | 1.00 | 21.79 | E |
| ATOM | 4777 | CA   | PHE | E | 47 | 82.192 | 20.595 | 10.599 | 1.00 | 22.22 | E |
| ATOM | 4778 | CB   | PHE | E | 47 | 83.175 | 19.864 | 11.515 | 1.00 | 22.30 | E |
| ATOM | 4779 | CG   | PHE | E | 47 | 83.058 | 20.249 | 12.968 | 1.00 | 22.20 | E |
| ATOM | 4780 | CD1  | PHE | E | 47 | 83.867 | 21.246 | 13.508 | 1.00 | 19.80 | E |
| ATOM | 4781 | CD2  | PHE | E | 47 | 82.151 | 19.598 | 13.802 | 1.00 | 23.06 | E |
| ATOM | 4782 | CE1  | PHE | E | 47 | 83.781 | 21.585 | 14.858 | 1.00 | 18.93 | E |
| ATOM | 4783 | CE2  | PHE | E | 47 | 82.055 | 19.931 | 15.157 | 1.00 | 22.63 | E |
| ATOM | 4784 | CZ   | PHE | E | 47 | 82.872 | 20.925 | 15.684 | 1.00 | 20.81 | E |
| ATOM | 4785 | C    | PHE | E | 47 | 82.513 | 20.278 | 9.147  | 1.00 | 24.14 | E |
| ATOM | 4786 | O    | PHE | E | 47 | 82.064 | 19.258 | 8.609  | 1.00 | 23.25 | E |
| ATOM | 4787 | N    | ARG | E | 48 | 83.272 | 21.164 | 8.511  | 1.00 | 22.66 | E |
| ATOM | 4788 | CA   | ARG | E | 48 | 83.672 | 20.966 | 7.131  | 1.00 | 23.86 | E |
| ATOM | 4789 | CB   | ARG | E | 48 | 82.801 | 21.795 | 6.181  | 1.00 | 23.48 | E |
| ATOM | 4790 | CG   | ARG | E | 48 | 81.339 | 21.375 | 6.091  | 1.00 | 25.01 | E |
| ATOM | 4791 | CD   | ARG | E | 48 | 81.155 | 20.061 | 5.348  | 1.00 | 25.08 | E |
| ATOM | 4792 | NE   | ARG | E | 48 | 79.747 | 19.811 | 5.044  | 1.00 | 27.17 | E |
| ATOM | 4793 | CZ   | ARG | E | 48 | 79.038 | 20.515 | 4.164  | 1.00 | 29.38 | E |
| ATOM | 4794 | NH1  | ARG | E | 48 | 79.604 | 21.513 | 3.498  | 1.00 | 31.36 | E |
| ATOM | 4795 | NH2  | ARG | E | 48 | 77.763 | 20.226 | 3.946  | 1.00 | 30.50 | E |
| ATOM | 4796 | C    | ARG | E | 48 | 85.119 | 21.395 | 6.972  | 1.00 | 24.13 | E |
| ATOM | 4797 | O    | ARG | E | 48 | 85.507 | 22.480 | 7.416  | 1.00 | 25.58 | E |
| ATOM | 4798 | N    | ALA | E | 49 | 85.924 | 20.537 | 6.360  | 1.00 | 22.26 | E |
| ATOM | 4799 | CA   | ALA | E | 49 | 87.316 | 20.875 | 6.122  | 1.00 | 23.11 | E |
| ATOM | 4800 | CB   | ALA | E | 49 | 88.102 | 19.630 | 5.711  | 1.00 | 22.46 | E |
| ATOM | 4801 | C    | ALA | E | 49 | 87.290 | 21.875 | 4.980  | 1.00 | 22.04 | E |
| ATOM | 4802 | O    | ALA | E | 49 | 86.507 | 21.722 | 4.048  | 1.00 | 23.16 | E |
| ATOM | 4803 | N    | VAL | E | 50 | 88.108 | 22.916 | 5.050  | 1.00 | 23.56 | E |
| ATOM | 4804 | CA   | VAL | E | 50 | 88.135 | 23.875 | 3.953  | 1.00 | 23.79 | E |
| ATOM | 4805 | CB   | VAL | E | 50 | 88.059 | 25.360 | 4.478  | 1.00 | 24.14 | E |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 4806 | CG1 | VAL | E | 50 | 88.341 | 25.408 | 5.959 | 1.00 24.71 | E |
| ATOM | 4807 | CG2 | VAL | E | 50 | 89.010 | 26.268 | 3.704 | 1.00 22.47 | E |
| ATOM | 4808 | C | VAL | E | 50 | 89.374 | 23.578 | 3.098 | 1.00 23.50 | E |
| ATOM | 4809 | O | VAL | E | 50 | 89.485 | 24.041 | 1.963 | 1.00 24.92 | E |
| ATOM | 4810 | N | THR | E | 51 | 90.281 | 22.770 | 3.650 | 1.00 24.49 | E |
| ATOM | 4811 | CA | THR | E | 51 | 91.492 | 22.317 | 2.951 | 1.00 25.50 | E |
| ATOM | 4812 | CB | THR | E | 51 | 92.742 | 23.198 | 3.234 | 1.00 25.69 | E |
| ATOM | 4813 | OG1 | THR | E | 51 | 93.171 | 23.007 | 4.586 | 1.00 27.89 | E |
| ATOM | 4814 | CG2 | THR | E | 51 | 92.443 | 24.670 | 2.985 | 1.00 23.29 | E |
| ATOM | 4815 | C | THR | E | 51 | 91.817 | 20.895 | 3.420 | 1.00 26.59 | E |
| ATOM | 4816 | O | THR | E | 51 | 91.387 | 20.477 | 4.496 | 1.00 27.35 | E |
| ATOM | 4817 | N | LEU | E | 52 | 92.576 | 20.154 | 2.617 | 1.00 28.03 | E |
| ATOM | 4818 | CA | LEU | E | 52 | 92.949 | 18.783 | 2.956 | 1.00 28.49 | E |
| ATOM | 4819 | CB | LEU | E | 52 | 93.995 | 18.259 | 1.969 | 1.00 30.33 | E |
| ATOM | 4820 | CG | LEU | E | 52 | 93.536 | 17.892 | 0.556 | 1.00 34.17 | E |
| ATOM | 4821 | CD1 | LEU | E | 52 | 94.749 | 17.628 | -0.334 | 1.00 34.41 | E |
| ATOM | 4822 | CD2 | LEU | E | 52 | 92.644 | 16.668 | 0.620 | 1.00 34.30 | E |
| ATOM | 4823 | C | LEU | E | 52 | 93.494 | 18.645 | 4.374 | 1.00 28.20 | E |
| ATOM | 4824 | O | LEU | E | 52 | 93.304 | 17.624 | 5.027 | 1.00 29.17 | E |
| ATOM | 4825 | N | LEU | E | 53 | 94.179 | 19.677 | 4.839 | 1.00 28.30 | E |
| ATOM | 4826 | CA | LEU | E | 53 | 94.766 | 19.682 | 6.171 | 1.00 28.75 | E |
| ATOM | 4827 | CB | LEU | E | 53 | 95.490 | 21.015 | 6.387 | 1.00 30.37 | E |
| ATOM | 4828 | CG | LEU | E | 53 | 96.939 | 21.010 | 6.882 | 1.00 32.74 | E |
| ATOM | 4829 | CD1 | LEU | E | 53 | 97.777 | 20.085 | 6.008 | 1.00 31.60 | E |
| ATOM | 4830 | CD2 | LEU | E | 53 | 97.498 | 22.444 | 6.854 | 1.00 30.06 | E |
| ATOM | 4831 | C | LEU | E | 53 | 93.727 | 19.464 | 7.278 | 1.00 27.82 | E |
| ATOM | 4832 | O | LEU | E | 53 | 94.027 | 18.858 | 8.312 | 1.00 25.47 | E |
| ATOM | 4833 | N | GLY | E | 54 | 92.508 | 19.957 | 7.059 | 1.00 27.39 | E |
| ATOM | 4834 | CA | GLY | E | 54 | 91.466 | 19.813 | 8.062 | 1.00 26.92 | E |
| ATOM | 4835 | C | GLY | E | 54 | 90.569 | 18.589 | 7.949 | 1.00 28.33 | E |
| ATOM | 4836 | O | GLY | E | 54 | 89.725 | 18.348 | 8.813 | 1.00 28.02 | E |
| ATOM | 4837 | N | LEU | E | 55 | 90.755 | 17.801 | 6.898 | 1.00 29.28 | E |
| ATOM | 4838 | CA | LEU | E | 55 | 89.930 | 16.620 | 6.675 | 1.00 31.43 | E |
| ATOM | 4839 | CB | LEU | E | 55 | 90.410 | 15.885 | 5.419 | 1.00 32.39 | E |
| ATOM | 4840 | CG | LEU | E | 55 | 89.426 | 14.934 | 4.731 | 1.00 35.68 | E |
| ATOM | 4841 | CD1 | LEU | E | 55 | 88.086 | 15.627 | 4.504 | 1.00 34.41 | E |
| ATOM | 4842 | CD2 | LEU | E | 55 | 90.018 | 14.473 | 3.406 | 1.00 35.99 | E |
| ATOM | 4843 | C | LEU | E | 55 | 89.865 | 15.659 | 7.867 | 1.00 32.09 | E |
| ATOM | 4844 | O | LEU | E | 55 | 88.778 | 15.294 | 8.312 | 1.00 32.58 | E |
| ATOM | 4845 | N | PRO | E | 56 | 91.023 | 15.235 | 8.402 | 1.00 31.67 | E |
| ATOM | 4846 | CD | PRO | E | 56 | 92.411 | 15.520 | 8.000 | 1.00 31.37 | E |
| ATOM | 4847 | CA | PRO | E | 56 | 90.986 | 14.316 | 9.546 | 1.00 31.17 | E |
| ATOM | 4848 | CB | PRO | E | 56 | 92.459 | 14.163 | 9.919 | 1.00 30.50 | E |
| ATOM | 4849 | CG | PRO | E | 56 | 93.161 | 14.352 | 8.611 | 1.00 31.19 | E |
| ATOM | 4850 | C | PRO | E | 56 | 90.158 | 14.865 | 10.708 | 1.00 31.43 | E |
| ATOM | 4851 | O | PRO | E | 56 | 89.250 | 14.195 | 11.205 | 1.00 32.17 | E |
| ATOM | 4852 | N | ALA | E | 57 | 90.473 | 16.086 | 11.138 | 1.00 29.94 | E |
| ATOM | 4853 | CA | ALA | E | 57 | 89.748 | 16.709 | 12.244 | 1.00 28.45 | E |
| ATOM | 4854 | CB | ALA | E | 57 | 90.314 | 18.098 | 12.532 | 1.00 27.09 | E |
| ATOM | 4855 | C | ALA | E | 57 | 88.249 | 16.807 | 11.960 | 1.00 27.57 | E |
| ATOM | 4856 | O | ALA | E | 57 | 87.436 | 16.466 | 12.812 | 1.00 26.57 | E |
| ATOM | 4857 | N | ALA | E | 58 | 87.899 | 17.270 | 10.761 | 1.00 27.40 | E |
| ATOM | 4858 | CA | ALA | E | 58 | 86.505 | 17.422 | 10.349 | 1.00 28.85 | E |
| ATOM | 4859 | CB | ALA | E | 58 | 86.439 | 18.007 | 8.939 | 1.00 27.80 | E |
| ATOM | 4860 | C | ALA | E | 58 | 85.726 | 16.110 | 10.406 | 1.00 30.37 | E |
| ATOM | 4861 | O | ALA | E | 58 | 84.624 | 16.058 | 10.954 | 1.00 29.58 | E |
| ATOM | 4862 | N | GLU | E | 59 | 86.292 | 15.052 | 9.837 | 1.00 32.24 | E |
| ATOM | 4863 | CA | GLU | E | 59 | 85.632 | 13.750 | 9.845 | 1.00 35.22 | E |
| ATOM | 4864 | CB | GLU | E | 59 | 86.441 | 12.724 | 9.049 | 1.00 36.81 | E |
| ATOM | 4865 | CG | GLU | E | 59 | 86.392 | 12.917 | 7.549 | 1.00 40.89 | E |
| ATOM | 4866 | CD | GLU | E | 59 | 87.057 | 11.775 | 6.805 | 1.00 44.28 | E |
| ATOM | 4867 | OE1 | GLU | E | 59 | 88.291 | 11.597 | 6.955 | 1.00 45.76 | E |
| ATOM | 4868 | OE2 | GLU | E | 59 | 86.342 | 11.052 | 6.075 | 1.00 45.12 | E |
| ATOM | 4869 | C | GLU | E | 59 | 85.441 | 13.231 | 11.260 | 1.00 34.08 | E |
| ATOM | 4870 | O | GLU | E | 59 | 84.384 | 12.697 | 11.596 | 1.00 34.48 | E |
| ATOM | 4871 | N | TYR | E | 60 | 86.466 | 13.387 | 12.090 | 1.00 33.21 | E |
| ATOM | 4872 | CA | TYR | E | 60 | 86.390 | 12.919 | 13.463 | 1.00 32.36 | E |
| ATOM | 4873 | CB | TYR | E | 60 | 87.724 | 13.101 | 14.177 | 1.00 33.78 | E |
| ATOM | 4874 | CG | TYR | E | 60 | 87.657 | 12.617 | 15.594 | 1.00 35.68 | E |
| ATOM | 4875 | CD1 | TYR | E | 60 | 87.543 | 11.259 | 15.872 | 1.00 37.48 | E |
| ATOM | 4876 | CE1 | TYR | E | 60 | 87.394 | 10.802 | 17.173 | 1.00 41.14 | E |
| ATOM | 4877 | CD2 | TYR | E | 60 | 87.628 | 13.514 | 16.655 | 1.00 37.26 | E |
| ATOM | 4878 | CE2 | TYR | E | 60 | 87.478 | 13.073 | 17.965 | 1.00 40.26 | E |
| ATOM | 4879 | CZ | TYR | E | 60 | 87.360 | 11.714 | 18.218 | 1.00 41.88 | E |

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ATOM   4880  OH  TYR E  60      87.198  11.262  19.508  1.00 44.51      E
ATOM   4881  C   TYR E  60      85.312  13.623  14.275  1.00 32.30      E
ATOM   4882  O   TYR E  60      84.430  12.976  14.839  1.00 30.56      E
ATOM   4883  N   TRP E  61      85.391  14.950  14.347  1.00 31.42      E
ATOM   4884  CA  TRP E  61      84.412  15.715  15.112  1.00 31.35      E
ATOM   4885  CB  TRP E  61      84.744  17.219  15.071  1.00 32.78      E
ATOM   4886  CG  TRP E  61      86.051  17.584  15.748  1.00 35.14      E
ATOM   4887  CD2 TRP E  61      86.909  18.687  15.425  1.00 37.07      E
ATOM   4888  CE2 TRP E  61      87.994  18.655  16.331  1.00 37.15      E
ATOM   4889  CE3 TRP E  61      86.864  19.706  14.458  1.00 39.50      E
ATOM   4890  CD1 TRP E  61      86.635  16.947  16.809  1.00 35.82      E
ATOM   4891  NE1 TRP E  61      87.800  17.582  17.163  1.00 35.66      E
ATOM   4892  CZ2 TRP E  61      89.034  19.602  16.300  1.00 38.95      E
ATOM   4893  CZ3 TRP E  61      87.902  20.656  14.427  1.00 41.16      E
ATOM   4894  CH2 TRP E  61      88.971  20.591  15.346  1.00 40.81      E
ATOM   4895  C   TRP E  61      82.968  15.472  14.653  1.00 29.29      E
ATOM   4896  O   TRP E  61      82.045  15.563  15.458  1.00 29.20      E
ATOM   4897  N   ASN E  62      82.772  15.162  13.373  1.00 27.86      E
ATOM   4898  CA  ASN E  62      81.428  14.902  12.853  1.00 29.09      E
ATOM   4899  CB  ASN E  62      81.379  15.051  11.331  1.00 29.42      E
ATOM   4900  CG  ASN E  62      81.241  16.492  10.893  1.00 31.22      E
ATOM   4901  OD1 ASN E  62      80.563  17.288  11.545  1.00 29.56      E
ATOM   4902  ND2 ASN E  62      81.870  16.834   9.772  1.00 31.73      E
ATOM   4903  C   ASN E  62      80.906  13.519  13.220  1.00 28.26      E
ATOM   4904  O   ASN E  62      79.716  13.242  13.086  1.00 27.48      E
ATOM   4905  N   SER E  63      81.795  12.647  13.672  1.00 27.47      E
ATOM   4906  CA  SER E  63      81.381  11.311  14.056  1.00 29.39      E
ATOM   4907  CB  SER E  63      82.511  10.310  13.803  1.00 28.56      E
ATOM   4908  OG  SER E  63      83.607  10.545  14.671  1.00 32.72      E
ATOM   4909  C   SER E  63      80.987  11.310  15.534  1.00 30.11      E
ATOM   4910  O   SER E  63      80.515  10.297  16.055  1.00 31.52      E
ATOM   4911  N   GLN E  64      81.173  12.453  16.196  1.00 28.86      E
ATOM   4912  CA  GLN E  64      80.834  12.604  17.612  1.00 28.28      E
ATOM   4913  CB  GLN E  64      81.929  13.379  18.350  1.00 29.50      E
ATOM   4914  CG  GLN E  64      83.330  12.787  18.266  1.00 29.72      E
ATOM   4915  CD  GLN E  64      83.418  11.412  18.888  1.00 32.69      E
ATOM   4916  OE1 GLN E  64      83.055  10.405  18.267  1.00 35.22      E
ATOM   4917  NE2 GLN E  64      83.887  11.358  20.128  1.00 31.92      E
ATOM   4918  C   GLN E  64      79.522  13.366  17.783  1.00 28.42      E
ATOM   4919  O   GLN E  64      79.525  14.599  17.800  1.00 27.68      E
ATOM   4920  N   LYS E  65      78.410  12.648  17.926  1.00 27.17      E
ATOM   4921  CA  LYS E  65      77.111  13.300  18.097  1.00 29.82      E
ATOM   4922  CB  LYS E  65      75.994  12.258  18.253  1.00 31.43      E
ATOM   4923  CG  LYS E  65      75.479  11.692  16.936  1.00 37.61      E
ATOM   4924  CD  LYS E  65      74.801  12.766  16.072  1.00 41.12      E
ATOM   4925  CE  LYS E  65      73.489  13.267  16.696  1.00 44.25      E
ATOM   4926  NZ  LYS E  65      72.832  14.322  15.861  1.00 44.10      E
ATOM   4927  C   LYS E  65      77.067  14.273  19.278  1.00 28.07      E
ATOM   4928  O   LYS E  65      76.406  15.308  19.211  1.00 27.46      E
ATOM   4929  N   ASP E  66      77.758  13.938  20.361  1.00 27.40      E
ATOM   4930  CA  ASP E  66      77.783  14.809  21.532  1.00 26.85      E
ATOM   4931  CB  ASP E  66      78.566  14.142  22.670  1.00 26.10      E
ATOM   4932  CG  ASP E  66      79.899  13.576  22.212  1.00 29.25      E
ATOM   4933  OD1 ASP E  66      79.915  12.836  21.205  1.00 28.95      E
ATOM   4934  OD2 ASP E  66      80.929  13.858  22.864  1.00 31.03      E
ATOM   4935  C   ASP E  66      78.390  16.174  21.193  1.00 26.21      E
ATOM   4936  O   ASP E  66      77.844  17.215  21.559  1.00 26.58      E
ATOM   4937  N   ILE E  67      79.510  16.170  20.478  1.00 26.25      E
ATOM   4938  CA  ILE E  67      80.164  17.414  20.100  1.00 25.76      E
ATOM   4939  CB  ILE E  67      81.551  17.153  19.477  1.00 27.31      E
ATOM   4940  CG2 ILE E  67      82.261  18.467  19.210  1.00 25.90      E
ATOM   4941  CG1 ILE E  67      82.396  16.304  20.429  1.00 28.85      E
ATOM   4942  CD1 ILE E  67      82.494  16.871  21.844  1.00 32.35      E
ATOM   4943  C   ILE E  67      79.307  18.189  19.108  1.00 25.95      E
ATOM   4944  O   ILE E  67      79.125  19.392  19.255  1.00 26.97      E
ATOM   4945  N   LEU E  68      78.775  17.504  18.100  1.00 26.05      E
ATOM   4946  CA  LEU E  68      77.927  18.172  17.113  1.00 26.36      E
ATOM   4947  CB  LEU E  68      77.382  17.169  16.094  1.00 26.91      E
ATOM   4948  CG  LEU E  68      78.154  16.987  14.790  1.00 27.01      E
ATOM   4949  CD1 LEU E  68      77.389  16.002  13.913  1.00 26.26      E
ATOM   4950  CD2 LEU E  68      78.311  18.342  14.076  1.00 24.04      E
ATOM   4951  C   LEU E  68      76.760  18.870  17.792  1.00 26.03      E
ATOM   4952  O   LEU E  68      76.433  20.011  17.465  1.00 25.76      E
ATOM   4953  N   GLU E  69      76.134  18.175  18.737  1.00 27.50      E
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| ATOM | 4954 | CA | GLU | E | 69 | 75.000 | 18.726 | 19.471 | 1.00 | 30.38 | E |
|------|------|------|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 4955 | CB | GLU | E | 69 | 74.481 | 17.720 | 20.508 | 1.00 | 34.06 | E |
| ATOM | 4956 | CG | GLU | E | 69 | 73.426 | 16.742 | 19.989 | 1.00 | 40.55 | E |
| ATOM | 4957 | CD | GLU | E | 69 | 72.211 | 17.444 | 19.392 | 1.00 | 44.43 | E |
| ATOM | 4958 | OE1 | GLU | E | 69 | 71.802 | 18.505 | 19.922 | 1.00 | 43.73 | E |
| ATOM | 4959 | OE2 | GLU | E | 69 | 71.656 | 16.926 | 18.397 | 1.00 | 48.15 | E |
| ATOM | 4960 | C | GLU | E | 69 | 75.335 | 20.034 | 20.178 | 1.00 | 29.17 | E |
| ATOM | 4961 | O | GLU | E | 69 | 74.587 | 21.009 | 20.071 | 1.00 | 29.71 | E |
| ATOM | 4962 | N | ARG | E | 70 | 76.453 | 20.059 | 20.899 | 1.00 | 26.65 | E |
| ATOM | 4963 | CA | ARG | E | 70 | 76.844 | 21.262 | 21.620 | 1.00 | 25.51 | E |
| ATOM | 4964 | CB | ARG | E | 70 | 78.001 | 20.965 | 22.572 | 1.00 | 27.14 | E |
| ATOM | 4965 | CG | ARG | E | 70 | 77.711 | 19.855 | 23.563 | 1.00 | 31.22 | E |
| ATOM | 4966 | CD | ARG | E | 70 | 78.637 | 19.934 | 24.769 | 1.00 | 35.11 | E |
| ATOM | 4967 | NE | ARG | E | 70 | 78.758 | 18.647 | 25.440 | 1.00 | 39.19 | E |
| ATOM | 4968 | CZ | ARG | E | 70 | 79.456 | 17.628 | 24.956 | 1.00 | 41.08 | E |
| ATOM | 4969 | NH1 | ARG | E | 70 | 80.096 | 17.752 | 23.802 | 1.00 | 45.32 | E |
| ATOM | 4970 | NH2 | ARG | E | 70 | 79.511 | 16.486 | 25.618 | 1.00 | 44.01 | E |
| ATOM | 4971 | C | ARG | E | 70 | 77.230 | 22.395 | 20.677 | 1.00 | 24.57 | E |
| ATOM | 4972 | O | ARG | E | 70 | 76.927 | 23.557 | 20.941 | 1.00 | 21.44 | E |
| ATOM | 4973 | N | LYS | E | 71 | 77.897 | 22.057 | 19.576 | 1.00 | 24.56 | E |
| ATOM | 4974 | CA | LYS | E | 71 | 78.309 | 23.071 | 18.612 | 1.00 | 24.08 | E |
| ATOM | 4975 | CB | LYS | E | 71 | 79.202 | 22.452 | 17.534 | 1.00 | 25.39 | E |
| ATOM | 4976 | CG | LYS | E | 71 | 80.100 | 23.474 | 16.852 | 1.00 | 29.73 | E |
| ATOM | 4977 | CD | LYS | E | 71 | 81.067 | 24.095 | 17.862 | 1.00 | 30.94 | E |
| ATOM | 4978 | CE | LYS | E | 71 | 81.905 | 25.205 | 17.256 | 1.00 | 31.82 | E |
| ATOM | 4979 | NZ | LYS | E | 71 | 82.774 | 25.849 | 18.290 | 1.00 | 33.45 | E |
| ATOM | 4980 | C | LYS | E | 71 | 77.087 | 23.732 | 17.960 | 1.00 | 22.42 | E |
| ATOM | 4981 | O | LYS | E | 71 | 77.045 | 24.951 | 17.780 | 1.00 | 18.65 | E |
| ATOM | 4982 | N | ARG | E | 72 | 76.092 | 22.919 | 17.620 | 1.00 | 22.31 | E |
| ATOM | 4983 | CA | ARG | E | 72 | 74.867 | 23.419 | 17.002 | 1.00 | 21.44 | E |
| ATOM | 4984 | CB | ARG | E | 72 | 73.984 | 22.250 | 16.578 | 1.00 | 19.93 | E |
| ATOM | 4985 | CG | ARG | E | 72 | 74.534 | 21.497 | 15.407 | 1.00 | 21.45 | E |
| ATOM | 4986 | CD | ARG | E | 72 | 73.779 | 20.223 | 15.141 | 1.00 | 23.34 | E |
| ATOM | 4987 | NE | ARG | E | 72 | 74.211 | 19.643 | 13.877 | 1.00 | 24.99 | E |
| ATOM | 4988 | CZ | ARG | E | 72 | 74.028 | 18.377 | 13.522 | 1.00 | 27.42 | E |
| ATOM | 4989 | NH1 | ARG | E | 72 | 73.411 | 17.533 | 14.344 | 1.00 | 25.90 | E |
| ATOM | 4990 | NH2 | ARG | E | 72 | 74.475 | 17.955 | 12.341 | 1.00 | 25.41 | E |
| ATOM | 4991 | C | ARG | E | 72 | 74.093 | 24.315 | 17.961 | 1.00 | 21.34 | E |
| ATOM | 4992 | O | ARG | E | 72 | 73.336 | 25.182 | 17.535 | 1.00 | 23.67 | E |
| ATOM | 4993 | N | ALA | E | 73 | 74.293 | 24.105 | 19.256 | 1.00 | 21.13 | E |
| ATOM | 4994 | CA | ALA | E | 73 | 73.610 | 24.887 | 20.281 | 1.00 | 22.11 | E |
| ATOM | 4995 | CB | ALA | E | 73 | 73.476 | 24.052 | 21.568 | 1.00 | 21.20 | E |
| ATOM | 4996 | C | ALA | E | 73 | 74.347 | 26.189 | 20.576 | 1.00 | 22.67 | E |
| ATOM | 4997 | O | ALA | E | 73 | 73.773 | 27.133 | 21.125 | 1.00 | 25.58 | E |
| ATOM | 4998 | N | ALA | E | 74 | 75.614 | 26.248 | 20.195 | 1.00 | 22.52 | E |
| ATOM | 4999 | CA | ALA | E | 74 | 76.420 | 27.432 | 20.448 | 1.00 | 22.20 | E |
| ATOM | 5000 | CB | ALA | E | 74 | 77.830 | 27.219 | 19.910 | 1.00 | 24.81 | E |
| ATOM | 5001 | C | ALA | E | 74 | 75.828 | 28.722 | 19.882 | 1.00 | 22.28 | E |
| ATOM | 5002 | O | ALA | E | 74 | 76.027 | 29.796 | 20.452 | 1.00 | 20.24 | E |
| ATOM | 5003 | N | VAL | E | 75 | 75.102 | 28.634 | 18.770 | 1.00 | 21.92 | E |
| ATOM | 5004 | CA | VAL | E | 75 | 74.519 | 29.841 | 18.185 | 1.00 | 21.69 | E |
| ATOM | 5005 | CB | VAL | E | 75 | 73.700 | 29.517 | 16.890 | 1.00 | 22.61 | E |
| ATOM | 5006 | CG1 | VAL | E | 75 | 72.488 | 28.657 | 17.219 | 1.00 | 24.39 | E |
| ATOM | 5007 | CG2 | VAL | E | 75 | 73.270 | 30.798 | 16.218 | 1.00 | 24.00 | E |
| ATOM | 5008 | C | VAL | E | 75 | 73.639 | 30.558 | 19.219 | 1.00 | 21.26 | E |
| ATOM | 5009 | O | VAL | E | 75 | 73.464 | 31.777 | 19.164 | 1.00 | 20.64 | E |
| ATOM | 5010 | N | ASP | E | 76 | 73.106 | 29.802 | 20.171 | 1.00 | 20.84 | E |
| ATOM | 5011 | CA | ASP | E | 76 | 72.273 | 30.385 | 21.220 | 1.00 | 23.98 | E |
| ATOM | 5012 | CB | ASP | E | 76 | 71.022 | 29.532 | 21.471 | 1.00 | 25.33 | E |
| ATOM | 5013 | CG | ASP | E | 76 | 70.010 | 29.605 | 20.331 | 1.00 | 27.46 | E |
| ATOM | 5014 | OD1 | ASP | E | 76 | 69.807 | 30.697 | 19.763 | 1.00 | 29.45 | E |
| ATOM | 5015 | OD2 | ASP | E | 76 | 69.398 | 28.566 | 20.020 | 1.00 | 31.17 | E |
| ATOM | 5016 | C | ASP | E | 76 | 73.044 | 30.525 | 22.538 | 1.00 | 24.46 | E |
| ATOM | 5017 | O | ASP | E | 76 | 72.910 | 31.524 | 23.247 | 1.00 | 25.64 | E |
| ATOM | 5018 | N | ARG | E | 77 | 73.846 | 29.515 | 22.855 | 1.00 | 23.56 | E |
| ATOM | 5019 | CA | ARG | E | 77 | 74.627 | 29.486 | 24.085 | 1.00 | 22.99 | E |
| ATOM | 5020 | CB | ARG | E | 77 | 75.176 | 28.077 | 24.279 | 1.00 | 26.55 | E |
| ATOM | 5021 | CG | ARG | E | 77 | 75.848 | 27.806 | 25.607 | 1.00 | 33.45 | E |
| ATOM | 5022 | CD | ARG | E | 77 | 75.961 | 26.295 | 25.825 | 1.00 | 37.66 | E |
| ATOM | 5023 | NE | ARG | E | 77 | 74.639 | 25.666 | 25.883 | 1.00 | 40.99 | E |
| ATOM | 5024 | CZ | ARG | E | 77 | 74.423 | 24.352 | 25.862 | 1.00 | 43.13 | E |
| ATOM | 5025 | NH1 | ARG | E | 77 | 75.438 | 23.503 | 25.782 | 1.00 | 43.11 | E |
| ATOM | 5026 | NH2 | ARG | E | 77 | 73.183 | 23.885 | 25.914 | 1.00 | 44.93 | E |
| ATOM | 5027 | C | ARG | E | 77 | 75.763 | 30.509 | 24.078 | 1.00 | 23.23 | E |

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 5028 | O   | ARG | E | 77 | 76.162 | 31.022 | 25.129 | 1.00 | 23.14 | E |
| ATOM | 5029 | N   | VAL | E | 78 | 76.275 | 30.808 | 22.889 | 1.00 | 20.54 | E |
| ATOM | 5030 | CA  | VAL | E | 78 | 77.354 | 31.767 | 22.741 | 1.00 | 19.56 | E |
| ATOM | 5031 | CB  | VAL | E | 78 | 78.500 | 31.181 | 21.891 | 1.00 | 19.17 | E |
| ATOM | 5032 | CG1 | VAL | E | 78 | 79.612 | 32.208 | 21.724 | 1.00 | 17.69 | E |
| ATOM | 5033 | CG2 | VAL | E | 78 | 79.032 | 29.921 | 22.541 | 1.00 | 19.40 | E |
| ATOM | 5034 | C   | VAL | E | 78 | 76.888 | 33.075 | 22.093 | 1.00 | 19.95 | E |
| ATOM | 5035 | O   | VAL | E | 78 | 76.786 | 34.110 | 22.756 | 1.00 | 21.57 | E |
| ATOM | 5036 | N   | CYS | E | 79 | 76.595 | 33.021 | 20.799 | 1.00 | 17.88 | E |
| ATOM | 5037 | CA  | CYS | E | 79 | 76.181 | 34.205 | 20.059 | 1.00 | 17.48 | E |
| ATOM | 5038 | C   | CYS | E | 79 | 74.967 | 34.966 | 20.620 | 1.00 | 18.40 | E |
| ATOM | 5039 | O   | CYS | E | 79 | 75.087 | 36.146 | 20.967 | 1.00 | 16.69 | E |
| ATOM | 5040 | CB  | CYS | E | 79 | 75.946 | 33.847 | 18.592 | 1.00 | 17.30 | E |
| ATOM | 5041 | SG  | CYS | E | 79 | 77.361 | 33.071 | 17.722 | 1.00 | 27.04 | E |
| ATOM | 5042 | N   | ARG | E | 80 | 73.802 | 34.326 | 20.717 | 1.00 | 17.59 | E |
| ATOM | 5043 | CA  | ARG | E | 80 | 72.641 | 35.050 | 21.240 | 1.00 | 20.01 | E |
| ATOM | 5044 | CB  | ARG | E | 80 | 71.340 | 34.256 | 21.032 | 1.00 | 20.22 | E |
| ATOM | 5045 | CG  | ARG | E | 80 | 70.886 | 34.213 | 19.584 | 1.00 | 22.92 | E |
| ATOM | 5046 | CD  | ARG | E | 80 | 69.423 | 33.811 | 19.439 | 1.00 | 23.91 | E |
| ATOM | 5047 | NE  | ARG | E | 80 | 68.972 | 33.965 | 18.057 | 1.00 | 23.49 | E |
| ATOM | 5048 | CZ  | ARG | E | 80 | 69.206 | 33.089 | 17.082 | 1.00 | 25.16 | E |
| ATOM | 5049 | NH1 | ARG | E | 80 | 69.884 | 31.975 | 17.326 | 1.00 | 24.15 | E |
| ATOM | 5050 | NH2 | ARG | E | 80 | 68.778 | 33.336 | 15.851 | 1.00 | 25.51 | E |
| ATOM | 5051 | C   | ARG | E | 80 | 72.804 | 35.423 | 22.716 | 1.00 | 20.35 | E |
| ATOM | 5052 | O   | ARG | E | 80 | 72.317 | 36.464 | 23.153 | 1.00 | 17.98 | E |
| ATOM | 5053 | N   | HIS | E | 81 | 73.495 | 34.581 | 23.479 | 1.00 | 21.22 | E |
| ATOM | 5054 | CA  | HIS | E | 81 | 73.717 | 34.867 | 24.895 | 1.00 | 22.79 | E |
| ATOM | 5055 | CB  | HIS | E | 81 | 74.467 | 33.717 | 25.572 | 1.00 | 24.38 | E |
| ATOM | 5056 | CG  | HIS | E | 81 | 74.955 | 34.046 | 26.950 | 1.00 | 26.42 | E |
| ATOM | 5057 | CD2 | HIS | E | 81 | 76.188 | 34.381 | 27.404 | 1.00 | 26.61 | E |
| ATOM | 5058 | ND1 | HIS | E | 81 | 74.122 | 34.080 | 28.048 | 1.00 | 26.60 | E |
| ATOM | 5059 | CE1 | HIS | E | 81 | 74.819 | 34.420 | 29.117 | 1.00 | 25.75 | E |
| ATOM | 5060 | NE2 | HIS | E | 81 | 76.075 | 34.609 | 28.754 | 1.00 | 26.16 | E |
| ATOM | 5061 | C   | HIS | E | 81 | 74.531 | 36.146 | 25.060 | 1.00 | 21.41 | E |
| ATOM | 5062 | O   | HIS | E | 81 | 74.109 | 37.076 | 25.742 | 1.00 | 19.84 | E |
| ATOM | 5063 | N   | ASN | E | 82 | 75.700 | 36.188 | 24.426 | 1.00 | 22.13 | E |
| ATOM | 5064 | CA  | ASN | E | 82 | 76.568 | 37.361 | 24.535 | 1.00 | 21.51 | E |
| ATOM | 5065 | CB  | ASN | E | 82 | 77.927 | 37.111 | 23.864 | 1.00 | 18.47 | E |
| ATOM | 5066 | CG  | ASN | E | 82 | 78.702 | 35.982 | 24.515 | 1.00 | 18.09 | E |
| ATOM | 5067 | OD1 | ASN | E | 82 | 78.453 | 35.632 | 25.669 | 1.00 | 19.05 | E |
| ATOM | 5068 | ND2 | ASN | E | 82 | 79.656 | 35.409 | 23.777 | 1.00 | 15.06 | E |
| ATOM | 5069 | C   | ASN | E | 82 | 75.936 | 38.612 | 23.949 | 1.00 | 20.33 | E |
| ATOM | 5070 | O   | ASN | E | 82 | 76.212 | 39.716 | 24.412 | 1.00 | 22.84 | E |
| ATOM | 5071 | N   | TYR | E | 83 | 75.089 | 38.454 | 22.940 | 1.00 | 19.71 | E |
| ATOM | 5072 | CA  | TYR | E | 83 | 74.454 | 39.620 | 22.336 | 1.00 | 20.96 | E |
| ATOM | 5073 | CB  | TYR | E | 83 | 73.619 | 39.211 | 21.114 | 1.00 | 21.58 | E |
| ATOM | 5074 | CG  | TYR | E | 83 | 73.223 | 40.368 | 20.218 | 1.00 | 22.56 | E |
| ATOM | 5075 | CD1 | TYR | E | 83 | 72.047 | 41.090 | 20.439 | 1.00 | 23.70 | E |
| ATOM | 5076 | CE1 | TYR | E | 83 | 71.682 | 42.152 | 19.593 | 1.00 | 25.46 | E |
| ATOM | 5077 | CD2 | TYR | E | 83 | 74.027 | 40.736 | 19.140 | 1.00 | 22.35 | E |
| ATOM | 5078 | CE2 | TYR | E | 83 | 73.675 | 41.788 | 18.297 | 1.00 | 24.48 | E |
| ATOM | 5079 | CZ  | TYR | E | 83 | 72.508 | 42.491 | 18.523 | 1.00 | 26.06 | E |
| ATOM | 5080 | OH  | TYR | E | 83 | 72.185 | 43.524 | 17.671 | 1.00 | 28.63 | E |
| ATOM | 5081 | C   | TYR | E | 83 | 73.583 | 40.345 | 23.363 | 1.00 | 21.22 | E |
| ATOM | 5082 | O   | TYR | E | 83 | 73.399 | 41.557 | 23.276 | 1.00 | 21.25 | E |
| ATOM | 5083 | N   | GLN | E | 84 | 73.046 | 39.606 | 24.333 | 1.00 | 22.94 | E |
| ATOM | 5084 | CA  | GLN | E | 84 | 72.234 | 40.226 | 25.377 | 1.00 | 25.07 | E |
| ATOM | 5085 | CB  | GLN | E | 84 | 71.631 | 39.180 | 26.324 | 1.00 | 25.76 | E |
| ATOM | 5086 | CG  | GLN | E | 84 | 70.863 | 38.047 | 25.653 | 1.00 | 30.97 | E |
| ATOM | 5087 | CD  | GLN | E | 84 | 69.889 | 38.525 | 24.594 | 1.00 | 33.95 | E |
| ATOM | 5088 | OE1 | GLN | E | 84 | 69.055 | 39.401 | 24.840 | 1.00 | 36.35 | E |
| ATOM | 5089 | NE2 | GLN | E | 84 | 69.986 | 37.940 | 23.401 | 1.00 | 36.25 | E |
| ATOM | 5090 | C   | GLN | E | 84 | 73.158 | 41.145 | 26.174 | 1.00 | 25.41 | E |
| ATOM | 5091 | O   | GLN | E | 84 | 72.804 | 42.290 | 26.473 | 1.00 | 27.11 | E |
| ATOM | 5092 | N   | LEU | E | 85 | 74.344 | 40.637 | 26.510 | 1.00 | 24.17 | E |
| ATOM | 5093 | CA  | LEU | E | 85 | 75.330 | 41.413 | 27.256 | 1.00 | 26.47 | E |
| ATOM | 5094 | CB  | LEU | E | 85 | 76.601 | 40.590 | 27.515 | 1.00 | 26.91 | E |
| ATOM | 5095 | CG  | LEU | E | 85 | 76.485 | 39.202 | 28.161 | 1.00 | 29.65 | E |
| ATOM | 5096 | CD1 | LEU | E | 85 | 77.872 | 38.735 | 28.587 | 1.00 | 31.29 | E |
| ATOM | 5097 | CD2 | LEU | E | 85 | 75.564 | 39.247 | 29.365 | 1.00 | 32.27 | E |
| ATOM | 5098 | C   | LEU | E | 85 | 75.698 | 42.661 | 26.459 | 1.00 | 26.89 | E |
| ATOM | 5099 | O   | LEU | E | 85 | 75.762 | 43.757 | 27.004 | 1.00 | 28.24 | E |
| ATOM | 5100 | N   | GLU | E | 86 | 75.941 | 42.484 | 25.162 | 1.00 | 27.39 | E |
| ATOM | 5101 | CA  | GLU | E | 86 | 76.293 | 43.603 | 24.295 | 1.00 | 28.02 | E |

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ATOM   5102  CB  GLU E  86      76.492  43.126  22.852  1.00 26.60          E
ATOM   5103  CG  GLU E  86      77.524  42.026  22.672  1.00 30.65          E
ATOM   5104  CD  GLU E  86      78.942  42.457  23.024  1.00 31.17          E
ATOM   5105  OE1 GLU E  86      79.860  41.612  22.919  1.00 31.68          E
ATOM   5106  OE2 GLU E  86      79.139  43.631  23.402  1.00 31.77          E
ATOM   5107  C   GLU E  86      75.165  44.630  24.327  1.00 27.95          E
ATOM   5108  O   GLU E  86      75.407  45.834  24.257  1.00 24.30          E
ATOM   5109  N   LEU E  87      73.935  44.130  24.442  1.00 28.96          E
ATOM   5110  CA  LEU E  87      72.736  44.962  24.468  1.00 32.20          E
ATOM   5111  CB  LEU E  87      71.496  44.062  24.423  1.00 32.64          E
ATOM   5112  CG  LEU E  87      70.506  44.100  23.248  1.00 35.59          E
ATOM   5113  CD1 LEU E  87      71.101  44.734  21.997  1.00 35.24          E
ATOM   5114  CD2 LEU E  87      70.071  42.675  22.965  1.00 34.35          E
ATOM   5115  C   LEU E  87      72.669  45.893  25.686  1.00 33.33          E
ATOM   5116  O   LEU E  87      71.967  46.902  25.663  1.00 32.52          E
ATOM   5117  N   ARG E  88      73.401  45.560  26.745  1.00 35.06          E
ATOM   5118  CA  ARG E  88      73.399  46.389  27.948  1.00 37.29          E
ATOM   5119  CB  ARG E  88      73.348  45.524  29.215  1.00 39.69          E
ATOM   5120  CG  ARG E  88      72.471  44.275  29.158  1.00 43.37          E
ATOM   5121  CD  ARG E  88      72.441  43.592  30.529  1.00 45.38          E
ATOM   5122  NE  ARG E  88      71.846  42.257  30.499  1.00 48.76          E
ATOM   5123  CZ  ARG E  88      70.625  41.985  30.047  1.00 50.95          E
ATOM   5124  NH1 ARG E  88      69.854  42.958  29.579  1.00 52.23          E
ATOM   5125  NH2 ARG E  88      70.171  40.738  30.064  1.00 51.26          E
ATOM   5126  C   ARG E  88      74.670  47.225  28.010  1.00 37.36          E
ATOM   5127  O   ARG E  88      74.842  48.044  28.913  1.00 37.55          E
ATOM   5128  N   THR E  89      75.564  47.019  27.049  1.00 36.40          E
ATOM   5129  CA  THR E  89      76.834  47.731  27.055  1.00 34.93          E
ATOM   5130  CB  THR E  89      77.951  46.807  27.590  1.00 36.26          E
ATOM   5131  OG1 THR E  89      77.973  45.590  26.825  1.00 34.21          E
ATOM   5132  CG2 THR E  89      77.708  46.478  29.056  1.00 33.95          E
ATOM   5133  C   THR E  89      77.294  48.304  25.718  1.00 33.37          E
ATOM   5134  O   THR E  89      76.958  49.431  25.356  1.00 33.30          E
ATOM   5135  N   THR E  90      78.080  47.510  25.000  1.00 32.11          E
ATOM   5136  CA  THR E  90      78.639  47.895  23.712  1.00 30.45          E
ATOM   5137  CB  THR E  90      79.313  46.681  23.041  1.00 31.20          E
ATOM   5138  OG1 THR E  90      80.238  46.086  23.958  1.00 32.67          E
ATOM   5139  CG2 THR E  90      80.076  47.109  21.811  1.00 32.64          E
ATOM   5140  C   THR E  90      77.639  48.504  22.738  1.00 28.40          E
ATOM   5141  O   THR E  90      77.903  49.538  22.133  1.00 27.20          E
ATOM   5142  N   LEU E  91      76.489  47.864  22.582  1.00 29.83          E
ATOM   5143  CA  LEU E  91      75.482  48.361  21.655  1.00 29.52          E
ATOM   5144  CB  LEU E  91      74.474  47.252  21.354  1.00 27.50          E
ATOM   5145  CG  LEU E  91      75.091  46.101  20.550  1.00 26.15          E
ATOM   5146  CD1 LEU E  91      74.102  44.959  20.457  1.00 24.51          E
ATOM   5147  CD2 LEU E  91      75.487  46.593  19.157  1.00 23.04          E
ATOM   5148  C   LEU E  91      74.770  49.629  22.129  1.00 30.74          E
ATOM   5149  O   LEU E  91      73.994  50.228  21.382  1.00 31.46          E
ATOM   5150  N   GLN E  92      75.035  50.043  23.366  1.00 29.33          E
ATOM   5151  CA  GLN E  92      74.427  51.259  23.884  1.00 30.04          E
ATOM   5152  CB  GLN E  92      73.869  51.044  25.294  1.00 31.55          E
ATOM   5153  CG  GLN E  92      72.500  50.381  25.327  1.00 36.90          E
ATOM   5154  CD  GLN E  92      71.865  50.426  26.706  1.00 41.59          E
ATOM   5155  OE1 GLN E  92      70.760  49.920  26.911  1.00 43.76          E
ATOM   5156  NE2 GLN E  92      72.563  51.037  27.662  1.00 43.75          E
ATOM   5157  C   GLN E  92      75.430  52.409  23.898  1.00 28.45          E
ATOM   5158  O   GLN E  92      75.059  53.558  24.125  1.00 28.57          E
ATOM   5159  N   ARG E  93      76.699  52.098  23.650  1.00 26.37          E
ATOM   5160  CA  ARG E  93      77.737  53.127  23.633  1.00 26.74          E
ATOM   5161  CB  ARG E  93      79.112  52.513  23.340  1.00 24.84          E
ATOM   5162  CG  ARG E  93      80.260  53.525  23.217  1.00 20.15          E
ATOM   5163  CD  ARG E  93      81.569  52.801  22.894  1.00 20.06          E
ATOM   5164  NE  ARG E  93      82.718  53.685  22.729  1.00 15.27          E
ATOM   5165  CZ  ARG E  93      83.316  54.330  23.729  1.00 16.93          E
ATOM   5166  NH1 ARG E  93      82.875  54.197  24.973  1.00 17.82          E
ATOM   5167  NH2 ARG E  93      84.367  55.101  23.492  1.00 16.28          E
ATOM   5168  C   ARG E  93      77.428  54.173  22.576  1.00 28.26          E
ATOM   5169  O   ARG E  93      77.202  53.847  21.407  1.00 29.80          E
ATOM   5170  N   ARG E  94      77.411  55.431  22.995  1.00 28.24          E
ATOM   5171  CA  ARG E  94      77.159  56.529  22.084  1.00 29.74          E
ATOM   5172  CB  ARG E  94      75.661  56.855  22.053  1.00 32.88          E
ATOM   5173  CG  ARG E  94      74.912  55.941  21.086  1.00 36.76          E
ATOM   5174  CD  ARG E  94      73.402  56.055  21.163  1.00 40.38          E
ATOM   5175  NE  ARG E  94      72.758  55.304  20.080  1.00 44.16          E
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| ATOM | 5176 | CZ | ARG | E | 94 | 72.871 | 53.991 | 19.894 | 1.00 | 43.57 | E |
| ATOM | 5177 | NH1 | ARG | E | 94 | 73.602 | 53.259 | 20.720 | 1.00 | 45.04 | E |
| ATOM | 5178 | NH2 | ARG | E | 94 | 72.262 | 53.408 | 18.869 | 1.00 | 45.75 | E |
| ATOM | 5179 | C | ARG | E | 94 | 77.992 | 57.734 | 22.497 | 1.00 | 29.26 | E |
| ATOM | 5180 | O | ARG | E | 94 | 77.773 | 58.331 | 23.546 | 1.00 | 30.32 | E |
| ATOM | 5181 | N | VAL | E | 95 | 78.974 | 58.063 | 21.667 | 1.00 | 26.76 | E |
| ATOM | 5182 | CA | VAL | E | 95 | 79.859 | 59.188 | 21.936 | 1.00 | 25.75 | E |
| ATOM | 5183 | CB | VAL | E | 95 | 81.340 | 58.763 | 21.855 | 1.00 | 22.33 | E |
| ATOM | 5184 | CG1 | VAL | E | 95 | 82.244 | 59.914 | 22.287 | 1.00 | 19.80 | E |
| ATOM | 5185 | CG2 | VAL | E | 95 | 81.565 | 57.534 | 22.717 | 1.00 | 19.11 | E |
| ATOM | 5186 | C | VAL | E | 95 | 79.600 | 60.266 | 20.902 | 1.00 | 26.51 | E |
| ATOM | 5187 | O | VAL | E | 95 | 79.787 | 60.042 | 19.703 | 1.00 | 27.04 | E |
| ATOM | 5188 | N | GLU | E | 96 | 79.160 | 61.430 | 21.366 | 1.00 | 27.28 | E |
| ATOM | 5189 | CA | GLU | E | 96 | 78.870 | 62.536 | 20.466 | 1.00 | 28.16 | E |
| ATOM | 5190 | CB | GLU | E | 96 | 78.260 | 63.716 | 21.227 | 1.00 | 30.40 | E |
| ATOM | 5191 | CG | GLU | E | 96 | 76.965 | 63.396 | 21.952 | 1.00 | 34.36 | E |
| ATOM | 5192 | CD | GLU | E | 96 | 76.348 | 64.625 | 22.609 | 1.00 | 36.84 | E |
| ATOM | 5193 | OE1 | GLU | E | 96 | 75.295 | 64.478 | 23.272 | 1.00 | 38.81 | E |
| ATOM | 5194 | OE2 | GLU | E | 96 | 76.914 | 65.734 | 22.460 | 1.00 | 35.73 | E |
| ATOM | 5195 | C | GLU | E | 96 | 80.148 | 62.987 | 19.793 | 1.00 | 25.65 | E |
| ATOM | 5196 | O | GLU | E | 96 | 81.176 | 63.171 | 20.440 | 1.00 | 24.93 | E |
| ATOM | 5197 | N | PRO | E | 97 | 80.101 | 63.168 | 18.473 | 1.00 | 25.41 | E |
| ATOM | 5198 | CD | PRO | E | 97 | 78.977 | 62.979 | 17.539 | 1.00 | 24.36 | E |
| ATOM | 5199 | CA | PRO | E | 97 | 81.304 | 63.603 | 17.770 | 1.00 | 24.81 | E |
| ATOM | 5200 | CB | PRO | E | 97 | 80.927 | 63.416 | 16.306 | 1.00 | 24.85 | E |
| ATOM | 5201 | CG | PRO | E | 97 | 79.456 | 63.717 | 16.309 | 1.00 | 25.36 | E |
| ATOM | 5202 | C | PRO | E | 97 | 81.643 | 65.048 | 18.089 | 1.00 | 24.48 | E |
| ATOM | 5203 | O | PRO | E | 97 | 80.761 | 65.844 | 18.419 | 1.00 | 23.85 | E |
| ATOM | 5204 | N | THR | E | 98 | 82.927 | 65.377 | 18.025 | 1.00 | 22.82 | E |
| ATOM | 5205 | CA | THR | E | 98 | 83.340 | 66.748 | 18.244 | 1.00 | 24.12 | E |
| ATOM | 5206 | CB | THR | E | 98 | 84.679 | 66.852 | 19.019 | 1.00 | 26.31 | E |
| ATOM | 5207 | OG1 | THR | E | 98 | 85.744 | 66.355 | 18.205 | 1.00 | 34.47 | E |
| ATOM | 5208 | CG2 | THR | E | 98 | 84.623 | 66.049 | 20.302 | 1.00 | 23.83 | E |
| ATOM | 5209 | C | THR | E | 98 | 83.519 | 67.254 | 16.817 | 1.00 | 22.12 | E |
| ATOM | 5210 | O | THR | E | 98 | 84.162 | 66.601 | 15.993 | 1.00 | 21.35 | E |
| ATOM | 5211 | N | VAL | E | 99 | 82.923 | 68.400 | 16.516 | 1.00 | 21.99 | E |
| ATOM | 5212 | CA | VAL | E | 99 | 83.001 | 68.957 | 15.177 | 1.00 | 20.67 | E |
| ATOM | 5213 | CB | VAL | E | 99 | 81.585 | 69.217 | 14.619 | 1.00 | 19.57 | E |
| ATOM | 5214 | CG1 | VAL | E | 99 | 81.667 | 69.645 | 13.154 | 1.00 | 14.62 | E |
| ATOM | 5215 | CG2 | VAL | E | 99 | 80.732 | 67.944 | 14.766 | 1.00 | 15.20 | E |
| ATOM | 5216 | C | VAL | E | 99 | 83.814 | 70.240 | 15.158 | 1.00 | 22.05 | E |
| ATOM | 5217 | O | VAL | E | 99 | 83.524 | 71.194 | 15.884 | 1.00 | 22.27 | E |
| ATOM | 5218 | N | THR | E | 100 | 84.827 | 70.250 | 14.304 | 1.00 | 21.34 | E |
| ATOM | 5219 | CA | THR | E | 100 | 85.728 | 71.376 | 14.176 | 1.00 | 23.10 | E |
| ATOM | 5220 | CB | THR | E | 100 | 87.104 | 71.024 | 14.786 | 1.00 | 24.55 | E |
| ATOM | 5221 | OG1 | THR | E | 100 | 86.941 | 70.728 | 16.180 | 1.00 | 30.47 | E |
| ATOM | 5222 | CG2 | THR | E | 100 | 88.079 | 72.183 | 14.634 | 1.00 | 27.79 | E |
| ATOM | 5223 | C | THR | E | 100 | 85.934 | 71.777 | 12.722 | 1.00 | 23.36 | E |
| ATOM | 5224 | O | THR | E | 100 | 86.024 | 70.926 | 11.842 | 1.00 | 21.77 | E |
| ATOM | 5225 | N | ILE | E | 101 | 86.009 | 73.082 | 12.473 | 1.00 | 24.40 | E |
| ATOM | 5226 | CA | ILE | E | 101 | 86.236 | 73.584 | 11.124 | 1.00 | 25.31 | E |
| ATOM | 5227 | CB | ILE | E | 101 | 85.092 | 74.518 | 10.645 | 1.00 | 24.21 | E |
| ATOM | 5228 | CG2 | ILE | E | 101 | 85.398 | 75.044 | 9.245 | 1.00 | 22.51 | E |
| ATOM | 5229 | CG1 | ILE | E | 101 | 83.760 | 73.768 | 10.636 | 1.00 | 24.86 | E |
| ATOM | 5230 | CD1 | ILE | E | 101 | 82.584 | 74.635 | 10.197 | 1.00 | 25.22 | E |
| ATOM | 5231 | C | ILE | E | 101 | 87.538 | 74.372 | 11.116 | 1.00 | 26.66 | E |
| ATOM | 5232 | O | ILE | E | 101 | 87.859 | 75.065 | 12.074 | 1.00 | 26.18 | E |
| ATOM | 5233 | N | SER | E | 102 | 88.287 | 74.262 | 10.029 | 1.00 | 31.17 | E |
| ATOM | 5234 | CA | SER | E | 102 | 89.547 | 74.977 | 9.902 | 1.00 | 35.36 | E |
| ATOM | 5235 | CB | SER | E | 102 | 90.619 | 74.306 | 10.755 | 1.00 | 34.20 | E |
| ATOM | 5236 | OG | SER | E | 102 | 90.777 | 72.953 | 10.374 | 1.00 | 40.09 | E |
| ATOM | 5237 | C | SER | E | 102 | 89.976 | 74.979 | 8.448 | 1.00 | 36.82 | E |
| ATOM | 5238 | O | SER | E | 102 | 89.913 | 73.953 | 7.777 | 1.00 | 36.68 | E |
| ATOM | 5239 | N | PRO | E | 103 | 90.404 | 76.139 | 7.932 | 1.00 | 39.96 | E |
| ATOM | 5240 | CD | PRO | E | 103 | 90.458 | 77.473 | 8.553 | 1.00 | 40.07 | E |
| ATOM | 5241 | CA | PRO | E | 103 | 90.831 | 76.190 | 6.532 | 1.00 | 42.01 | E |
| ATOM | 5242 | CB | PRO | E | 103 | 90.856 | 77.682 | 6.237 | 1.00 | 41.76 | E |
| ATOM | 5243 | CG | PRO | E | 103 | 91.282 | 78.258 | 7.556 | 1.00 | 42.86 | E |
| ATOM | 5244 | C | PRO | E | 103 | 92.196 | 75.534 | 6.390 | 1.00 | 44.62 | E |
| ATOM | 5245 | O | PRO | E | 103 | 92.943 | 75.430 | 7.365 | 1.00 | 44.53 | E |
| ATOM | 5246 | N | SER | E | 104 | 92.514 | 75.086 | 5.181 | 1.00 | 47.92 | E |
| ATOM | 5247 | CA | SER | E | 104 | 93.789 | 74.426 | 4.920 | 1.00 | 50.83 | E |
| ATOM | 5248 | CB | SER | E | 104 | 93.712 | 73.637 | 3.612 | 1.00 | 52.33 | E |
| ATOM | 5249 | OG | SER | E | 104 | 94.904 | 72.901 | 3.396 | 1.00 | 55.60 | E |

| ATOM | 5250 | C | SER | E | 104 | 94.941 | 75.422 | 4.845 | 1.00 | 52.18 | E |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 5251 | O | SER | E | 104 | 96.080 | 75.093 | 5.186 | 1.00 | 53.53 | E |
| ATOM | 5252 | N | ASN | E | 113 | 90.669 | 78.112 | -1.692 | 1.00 | 48.40 | E |
| ATOM | 5253 | CA | ASN | E | 113 | 90.651 | 77.795 | -0.269 | 1.00 | 47.57 | E |
| ATOM | 5254 | CB | ASN | E | 113 | 89.863 | 78.854 | 0.496 | 1.00 | 51.34 | E |
| ATOM | 5255 | CG | ASN | E | 113 | 90.504 | 80.219 | 0.417 | 1.00 | 52.99 | E |
| ATOM | 5256 | OD1 | ASN | E | 113 | 90.693 | 80.765 | -0.670 | 1.00 | 55.11 | E |
| ATOM | 5257 | ND2 | ASN | E | 113 | 90.845 | 80.781 | 1.572 | 1.00 | 55.09 | E |
| ATOM | 5258 | C | ASN | E | 113 | 90.045 | 76.424 | -0.001 | 1.00 | 44.87 | E |
| ATOM | 5259 | O | ASN | E | 113 | 89.374 | 75.852 | -0.860 | 1.00 | 44.99 | E |
| ATOM | 5260 | N | LEU | E | 114 | 90.282 | 75.904 | 1.197 | 1.00 | 41.65 | E |
| ATOM | 5261 | CA | LEU | E | 114 | 89.765 | 74.592 | 1.568 | 1.00 | 38.53 | E |
| ATOM | 5262 | CB | LEU | E | 114 | 90.823 | 73.521 | 1.287 | 1.00 | 38.84 | E |
| ATOM | 5263 | CG | LEU | E | 114 | 90.383 | 72.060 | 1.441 | 1.00 | 40.32 | E |
| ATOM | 5264 | CD1 | LEU | E | 114 | 89.314 | 71.726 | 0.400 | 1.00 | 39.94 | E |
| ATOM | 5265 | CD2 | LEU | E | 114 | 91.586 | 71.145 | 1.266 | 1.00 | 40.52 | E |
| ATOM | 5266 | C | LEU | E | 114 | 89.349 | 74.523 | 3.036 | 1.00 | 34.78 | E |
| ATOM | 5267 | O | LEU | E | 114 | 90.173 | 74.684 | 3.929 | 1.00 | 33.51 | E |
| ATOM | 5268 | N | LEU | E | 115 | 88.063 | 74.293 | 3.278 | 1.00 | 32.05 | E |
| ATOM | 5269 | CA | LEU | E | 115 | 87.550 | 74.181 | 4.641 | 1.00 | 29.68 | E |
| ATOM | 5270 | CB | LEU | E | 115 | 86.158 | 74.809 | 4.754 | 1.00 | 29.84 | E |
| ATOM | 5271 | CG | LEU | E | 115 | 86.046 | 76.257 | 5.241 | 1.00 | 31.52 | E |
| ATOM | 5272 | CD1 | LEU | E | 115 | 87.101 | 77.140 | 4.574 | 1.00 | 32.51 | E |
| ATOM | 5273 | CD2 | LEU | E | 115 | 84.636 | 76.762 | 4.948 | 1.00 | 30.75 | E |
| ATOM | 5274 | C | LEU | E | 115 | 87.472 | 72.712 | 5.034 | 1.00 | 27.57 | E |
| ATOM | 5275 | O | LEU | E | 115 | 86.871 | 71.900 | 4.331 | 1.00 | 25.33 | E |
| ATOM | 5276 | N | VAL | E | 116 | 88.089 | 72.381 | 6.161 | 1.00 | 26.32 | E |
| ATOM | 5277 | CA | VAL | E | 116 | 88.099 | 71.014 | 6.651 | 1.00 | 24.42 | E |
| ATOM | 5278 | CB | VAL | E | 116 | 89.513 | 70.572 | 7.075 | 1.00 | 24.51 | E |
| ATOM | 5279 | CG1 | VAL | E | 116 | 89.467 | 69.160 | 7.641 | 1.00 | 22.66 | E |
| ATOM | 5280 | CG2 | VAL | E | 116 | 90.458 | 70.643 | 5.879 | 1.00 | 26.70 | E |
| ATOM | 5281 | C | VAL | E | 116 | 87.195 | 70.842 | 7.846 | 1.00 | 22.77 | E |
| ATOM | 5282 | O | VAL | E | 116 | 87.376 | 71.496 | 8.868 | 1.00 | 23.04 | E |
| ATOM | 5283 | N | CYS | E | 117 | 86.208 | 69.968 | 7.717 | 1.00 | 22.34 | E |
| ATOM | 5284 | CA | CYS | E | 117 | 85.326 | 69.711 | 8.840 | 1.00 | 21.65 | E |
| ATOM | 5285 | C | CYS | E | 117 | 85.769 | 68.391 | 9.466 | 1.00 | 19.44 | E |
| ATOM | 5286 | O | CYS | E | 117 | 85.607 | 67.319 | 8.877 | 1.00 | 18.95 | E |
| ATOM | 5287 | CB | CYS | E | 117 | 83.863 | 69.626 | 8.401 | 1.00 | 22.57 | E |
| ATOM | 5288 | SG | CYS | E | 117 | 82.771 | 69.420 | 9.844 | 1.00 | 25.79 | E |
| ATOM | 5289 | N | SER | E | 118 | 86.355 | 68.488 | 10.654 | 1.00 | 19.92 | E |
| ATOM | 5290 | CA | SER | E | 118 | 86.837 | 67.330 | 11.387 | 1.00 | 17.98 | E |
| ATOM | 5291 | CB | SER | E | 118 | 88.115 | 67.671 | 12.146 | 1.00 | 18.33 | E |
| ATOM | 5292 | OG | SER | E | 118 | 89.121 | 68.117 | 11.260 | 1.00 | 24.58 | E |
| ATOM | 5293 | C | SER | E | 118 | 85.798 | 66.860 | 12.377 | 1.00 | 17.01 | E |
| ATOM | 5294 | O | SER | E | 118 | 85.507 | 67.543 | 13.354 | 1.00 | 16.69 | E |
| ATOM | 5295 | N | VAL | E | 119 | 85.240 | 65.688 | 12.112 | 1.00 | 16.58 | E |
| ATOM | 5296 | CA | VAL | E | 119 | 84.242 | 65.095 | 12.985 | 1.00 | 16.03 | E |
| ATOM | 5297 | CB | VAL | E | 119 | 83.040 | 64.582 | 12.160 | 1.00 | 15.47 | E |
| ATOM | 5298 | CG1 | VAL | E | 119 | 81.918 | 64.147 | 13.077 | 1.00 | 13.75 | E |
| ATOM | 5299 | CG2 | VAL | E | 119 | 82.559 | 65.686 | 11.216 | 1.00 | 10.95 | E |
| ATOM | 5300 | C | VAL | E | 119 | 85.018 | 63.960 | 13.638 | 1.00 | 17.51 | E |
| ATOM | 5301 | O | VAL | E | 119 | 85.238 | 62.906 | 13.042 | 1.00 | 19.30 | E |
| ATOM | 5302 | N | THR | E | 120 | 85.442 | 64.203 | 14.871 | 1.00 | 18.44 | E |
| ATOM | 5303 | CA | THR | E | 120 | 86.265 | 63.266 | 15.616 | 1.00 | 18.41 | E |
| ATOM | 5304 | CB | THR | E | 120 | 87.562 | 63.962 | 16.042 | 1.00 | 18.11 | E |
| ATOM | 5305 | OG1 | THR | E | 120 | 87.242 | 65.078 | 16.887 | 1.00 | 17.18 | E |
| ATOM | 5306 | CG2 | THR | E | 120 | 88.304 | 64.481 | 14.835 | 1.00 | 16.77 | E |
| ATOM | 5307 | C | THR | E | 120 | 85.655 | 62.656 | 16.875 | 1.00 | 20.11 | E |
| ATOM | 5308 | O | THR | E | 120 | 84.665 | 63.148 | 17.417 | 1.00 | 21.96 | E |
| ATOM | 5309 | N | ASP | E | 121 | 86.272 | 61.566 | 17.319 | 1.00 | 19.96 | E |
| ATOM | 5310 | CA | ASP | E | 121 | 85.882 | 60.864 | 18.529 | 1.00 | 21.06 | E |
| ATOM | 5311 | CB | ASP | E | 121 | 86.313 | 61.686 | 19.745 | 1.00 | 25.93 | E |
| ATOM | 5312 | CG | ASP | E | 121 | 87.814 | 61.765 | 19.882 | 1.00 | 30.02 | E |
| ATOM | 5313 | OD1 | ASP | E | 121 | 88.291 | 62.524 | 20.756 | 1.00 | 34.97 | E |
| ATOM | 5314 | OD2 | ASP | E | 121 | 88.513 | 61.063 | 19.114 | 1.00 | 31.15 | E |
| ATOM | 5315 | C | ASP | E | 121 | 84.431 | 60.463 | 18.709 | 1.00 | 20.39 | E |
| ATOM | 5316 | O | ASP | E | 121 | 83.857 | 60.698 | 19.766 | 1.00 | 22.05 | E |
| ATOM | 5317 | N | PHE | E | 122 | 83.827 | 59.841 | 17.708 | 1.00 | 19.69 | E |
| ATOM | 5318 | CA | PHE | E | 122 | 82.443 | 59.429 | 17.873 | 1.00 | 18.28 | E |
| ATOM | 5319 | CB | PHE | E | 122 | 81.538 | 60.108 | 16.843 | 1.00 | 16.99 | E |
| ATOM | 5320 | CG | PHE | E | 122 | 81.905 | 59.821 | 15.417 | 1.00 | 16.67 | E |
| ATOM | 5321 | CD1 | PHE | E | 122 | 82.770 | 60.661 | 14.725 | 1.00 | 16.72 | E |
| ATOM | 5322 | CD2 | PHE | E | 122 | 81.370 | 58.717 | 14.756 | 1.00 | 17.17 | E |
| ATOM | 5323 | CE1 | PHE | E | 122 | 83.096 | 60.410 | 13.384 | 1.00 | 17.00 | E |

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| ATOM | 5324 | CE2 | PHE | E | 122 | 81.686 | 58.456 | 13.419 | 1.00 | 16.82 | E |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 5325 | CZ | PHE | E | 122 | 82.549 | 59.305 | 12.733 | 1.00 | 15.81 | E |
| ATOM | 5326 | C | PHE | E | 122 | 82.287 | 57.925 | 17.774 | 1.00 | 18.35 | E |
| ATOM | 5327 | O | PHE | E | 122 | 83.168 | 57.231 | 17.272 | 1.00 | 15.90 | E |
| ATOM | 5328 | N | TYR | E | 123 | 81.157 | 57.436 | 18.276 | 1.00 | 19.49 | E |
| ATOM | 5329 | CA | TYR | E | 123 | 80.818 | 56.021 | 18.243 | 1.00 | 20.92 | E |
| ATOM | 5330 | CB | TYR | E | 123 | 81.523 | 55.261 | 19.374 | 1.00 | 21.02 | E |
| ATOM | 5331 | CG | TYR | E | 123 | 81.387 | 53.762 | 19.247 | 1.00 | 20.05 | E |
| ATOM | 5332 | CD1 | TYR | E | 123 | 80.242 | 53.103 | 19.688 | 1.00 | 21.66 | E |
| ATOM | 5333 | CE1 | TYR | E | 123 | 80.095 | 51.726 | 19.516 | 1.00 | 21.85 | E |
| ATOM | 5334 | CD2 | TYR | E | 123 | 82.383 | 53.009 | 18.633 | 1.00 | 20.08 | E |
| ATOM | 5335 | CE2 | TYR | E | 123 | 82.250 | 51.643 | 18.455 | 1.00 | 19.20 | E |
| ATOM | 5336 | CZ | TYR | E | 123 | 81.105 | 51.002 | 18.896 | 1.00 | 22.24 | E |
| ATOM | 5337 | OH | TYR | E | 123 | 80.970 | 49.640 | 18.712 | 1.00 | 25.26 | E |
| ATOM | 5338 | C | TYR | E | 123 | 79.311 | 55.957 | 18.440 | 1.00 | 21.42 | E |
| ATOM | 5339 | O | TYR | E | 123 | 78.778 | 56.647 | 19.305 | 1.00 | 23.90 | E |
| ATOM | 5340 | N | PRO | E | 124 | 78.609 | 55.100 | 17.676 | 1.00 | 20.39 | E |
| ATOM | 5341 | CD | PRO | E | 124 | 77.155 | 54.937 | 17.844 | 1.00 | 21.24 | E |
| ATOM | 5342 | CA | PRO | E | 124 | 79.113 | 54.177 | 16.655 | 1.00 | 21.61 | E |
| ATOM | 5343 | CB | PRO | E | 124 | 77.956 | 53.188 | 16.500 | 1.00 | 19.35 | E |
| ATOM | 5344 | CG | PRO | E | 124 | 76.776 | 54.056 | 16.670 | 1.00 | 19.34 | E |
| ATOM | 5345 | C | PRO | E | 124 | 79.549 | 54.802 | 15.325 | 1.00 | 20.84 | E |
| ATOM | 5346 | O | PRO | E | 124 | 79.602 | 56.024 | 15.184 | 1.00 | 22.13 | E |
| ATOM | 5347 | N | ALA | E | 125 | 79.862 | 53.940 | 14.361 | 1.00 | 22.61 | E |
| ATOM | 5348 | CA | ALA | E | 125 | 80.329 | 54.341 | 13.027 | 1.00 | 25.48 | E |
| ATOM | 5349 | CB | ALA | E | 125 | 80.860 | 53.121 | 12.288 | 1.00 | 26.06 | E |
| ATOM | 5350 | C | ALA | E | 125 | 79.311 | 55.058 | 12.137 | 1.00 | 27.38 | E |
| ATOM | 5351 | O | ALA | E | 125 | 79.681 | 55.906 | 11.332 | 1.00 | 29.08 | E |
| ATOM | 5352 | N | GLN | E | 126 | 78.039 | 54.706 | 12.268 | 1.00 | 29.18 | E |
| ATOM | 5353 | CA | GLN | E | 126 | 76.990 | 55.312 | 11.455 | 1.00 | 29.94 | E |
| ATOM | 5354 | CB | GLN | E | 126 | 75.625 | 54.737 | 11.848 | 1.00 | 33.48 | E |
| ATOM | 5355 | CG | GLN | E | 126 | 75.536 | 53.200 | 11.840 | 1.00 | 39.27 | E |
| ATOM | 5356 | CD | GLN | E | 126 | 76.067 | 52.537 | 13.117 | 1.00 | 41.92 | E |
| ATOM | 5357 | OE1 | GLN | E | 126 | 77.271 | 52.523 | 13.379 | 1.00 | 44.02 | E |
| ATOM | 5358 | NE2 | GLN | E | 126 | 75.159 | 51.981 | 13.913 | 1.00 | 43.83 | E |
| ATOM | 5359 | C | GLN | E | 126 | 76.977 | 56.829 | 11.621 | 1.00 | 28.88 | E |
| ATOM | 5360 | O | GLN | E | 126 | 76.739 | 57.331 | 12.719 | 1.00 | 28.83 | E |
| ATOM | 5361 | N | ILE | E | 127 | 77.221 | 57.558 | 10.532 | 1.00 | 27.90 | E |
| ATOM | 5362 | CA | ILE | E | 127 | 77.245 | 59.018 | 10.591 | 1.00 | 25.67 | E |
| ATOM | 5363 | CB | ILE | E | 127 | 78.611 | 59.514 | 11.150 | 1.00 | 25.23 | E |
| ATOM | 5364 | CG2 | ILE | E | 127 | 79.693 | 59.398 | 10.084 | 1.00 | 21.16 | E |
| ATOM | 5365 | CG1 | ILE | E | 127 | 78.504 | 60.965 | 11.610 | 1.00 | 22.40 | E |
| ATOM | 5366 | CD1 | ILE | E | 127 | 79.610 | 61.376 | 12.546 | 1.00 | 25.35 | E |
| ATOM | 5367 | C | ILE | E | 127 | 76.985 | 59.673 | 9.230 | 1.00 | 26.38 | E |
| ATOM | 5368 | O | ILE | E | 127 | 77.196 | 59.065 | 8.182 | 1.00 | 26.20 | E |
| ATOM | 5369 | N | LYS | E | 128 | 76.521 | 60.916 | 9.252 | 1.00 | 25.64 | E |
| ATOM | 5370 | CA | LYS | E | 128 | 76.248 | 61.635 | 8.016 | 1.00 | 29.02 | E |
| ATOM | 5371 | CB | LYS | E | 128 | 74.754 | 61.566 | 7.671 | 1.00 | 29.97 | E |
| ATOM | 5372 | CG | LYS | E | 128 | 74.408 | 62.178 | 6.317 | 1.00 | 35.17 | E |
| ATOM | 5373 | CD | LYS | E | 128 | 75.175 | 61.487 | 5.183 | 1.00 | 39.63 | E |
| ATOM | 5374 | CE | LYS | E | 128 | 74.936 | 62.163 | 3.836 | 1.00 | 41.20 | E |
| ATOM | 5375 | NZ | LYS | E | 128 | 75.685 | 61.492 | 2.731 | 1.00 | 44.74 | E |
| ATOM | 5376 | C | LYS | E | 128 | 76.683 | 63.090 | 8.154 | 1.00 | 28.40 | E |
| ATOM | 5377 | O | LYS | E | 128 | 76.203 | 63.812 | 9.028 | 1.00 | 27.15 | E |
| ATOM | 5378 | N | VAL | E | 129 | 77.600 | 63.506 | 7.287 | 1.00 | 28.99 | E |
| ATOM | 5379 | CA | VAL | E | 129 | 78.119 | 64.866 | 7.304 | 1.00 | 29.32 | E |
| ATOM | 5380 | CB | VAL | E | 129 | 79.651 | 64.860 | 7.502 | 1.00 | 30.69 | E |
| ATOM | 5381 | CG1 | VAL | E | 129 | 80.171 | 66.282 | 7.654 | 1.00 | 27.54 | E |
| ATOM | 5382 | CG2 | VAL | E | 129 | 80.014 | 64.012 | 8.721 | 1.00 | 30.82 | E |
| ATOM | 5383 | C | VAL | E | 129 | 77.788 | 65.574 | 5.992 | 1.00 | 30.45 | E |
| ATOM | 5384 | O | VAL | E | 129 | 78.042 | 65.039 | 4.915 | 1.00 | 30.36 | E |
| ATOM | 5385 | N | ARG | E | 130 | 77.221 | 66.775 | 6.090 | 1.00 | 31.17 | E |
| ATOM | 5386 | CA | ARG | E | 130 | 76.851 | 67.562 | 4.914 | 1.00 | 32.17 | E |
| ATOM | 5387 | CB | ARG | E | 130 | 75.330 | 67.626 | 4.764 | 1.00 | 34.73 | E |
| ATOM | 5388 | CG | ARG | E | 130 | 74.632 | 66.335 | 4.400 | 1.00 | 40.85 | E |
| ATOM | 5389 | CD | ARG | E | 130 | 73.121 | 66.527 | 4.511 | 1.00 | 46.16 | E |
| ATOM | 5390 | NE | ARG | E | 130 | 72.365 | 65.456 | 3.864 | 1.00 | 51.33 | E |
| ATOM | 5391 | CZ | ARG | E | 130 | 71.046 | 65.308 | 3.959 | 1.00 | 53.45 | E |
| ATOM | 5392 | NH1 | ARG | E | 130 | 70.327 | 66.162 | 4.680 | 1.00 | 54.21 | E |
| ATOM | 5393 | NH2 | ARG | E | 130 | 70.444 | 64.307 | 3.329 | 1.00 | 53.97 | E |
| ATOM | 5394 | C | ARG | E | 130 | 77.359 | 68.994 | 5.017 | 1.00 | 30.88 | E |
| ATOM | 5395 | O | ARG | E | 130 | 77.321 | 69.590 | 6.093 | 1.00 | 30.84 | E |
| ATOM | 5396 | N | TRP | E | 131 | 77.831 | 69.542 | 3.900 | 1.00 | 29.14 | E |
| ATOM | 5397 | CA | TRP | E | 131 | 78.291 | 70.928 | 3.865 | 1.00 | 29.57 | E |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 5398 | CB | TRP | E | 131 | 79.538 | 71.086 | 2.996 | 1.00 | 27.97 | E |
| ATOM | 5399 | CG | TRP | E | 131 | 80.809 | 70.979 | 3.760 | 1.00 | 29.37 | E |
| ATOM | 5400 | CD2 | TRP | E | 131 | 81.342 | 71.949 | 4.671 | 1.00 | 29.95 | E |
| ATOM | 5401 | CE2 | TRP | E | 131 | 82.551 | 71.427 | 5.174 | 1.00 | 29.75 | E |
| ATOM | 5402 | CE3 | TRP | E | 131 | 80.913 | 73.209 | 5.111 | 1.00 | 30.39 | E |
| ATOM | 5403 | CD1 | TRP | E | 131 | 81.689 | 69.941 | 3.747 | 1.00 | 29.02 | E |
| ATOM | 5404 | NE1 | TRP | E | 131 | 82.738 | 70.200 | 4.592 | 1.00 | 30.01 | E |
| ATOM | 5405 | CZ2 | TRP | E | 131 | 83.340 | 72.119 | 6.095 | 1.00 | 28.79 | E |
| ATOM | 5406 | CZ3 | TRP | E | 131 | 81.697 | 73.900 | 6.027 | 1.00 | 31.30 | E |
| ATOM | 5407 | CH2 | TRP | E | 131 | 82.900 | 73.350 | 6.509 | 1.00 | 31.69 | E |
| ATOM | 5408 | C | TRP | E | 131 | 77.185 | 71.817 | 3.301 | 1.00 | 30.08 | E |
| ATOM | 5409 | O | TRP | E | 131 | 76.449 | 71.413 | 2.392 | 1.00 | 29.15 | E |
| ATOM | 5410 | N | PHE | E | 132 | 77.081 | 73.027 | 3.842 | 1.00 | 29.87 | E |
| ATOM | 5411 | CA | PHE | E | 132 | 76.078 | 73.985 | 3.405 | 1.00 | 30.98 | E |
| ATOM | 5412 | CB | PHE | E | 132 | 74.963 | 74.094 | 4.443 | 1.00 | 32.09 | E |
| ATOM | 5413 | CG | PHE | E | 132 | 74.041 | 72.918 | 4.461 | 1.00 | 33.03 | E |
| ATOM | 5414 | CD1 | PHE | E | 132 | 72.913 | 72.896 | 3.650 | 1.00 | 35.25 | E |
| ATOM | 5415 | CD2 | PHE | E | 132 | 74.306 | 71.822 | 5.273 | 1.00 | 33.31 | E |
| ATOM | 5416 | CE1 | PHE | E | 132 | 72.055 | 71.794 | 3.646 | 1.00 | 35.49 | E |
| ATOM | 5417 | CE2 | PHE | E | 132 | 73.460 | 70.717 | 5.279 | 1.00 | 35.47 | E |
| ATOM | 5418 | CZ | PHE | E | 132 | 72.330 | 70.704 | 4.461 | 1.00 | 35.97 | E |
| ATOM | 5419 | C | PHE | E | 132 | 76.668 | 75.364 | 3.182 | 1.00 | 32.06 | E |
| ATOM | 5420 | O | PHE | E | 132 | 77.537 | 75.812 | 3.929 | 1.00 | 29.15 | E |
| ATOM | 5421 | N | ARG | E | 133 | 76.186 | 76.026 | 2.138 | 1.00 | 34.68 | E |
| ATOM | 5422 | CA | ARG | E | 133 | 76.613 | 77.375 | 1.809 | 1.00 | 37.78 | E |
| ATOM | 5423 | CB | ARG | E | 133 | 77.281 | 77.420 | 0.434 | 1.00 | 40.14 | E |
| ATOM | 5424 | CG | ARG | E | 133 | 77.755 | 78.810 | 0.005 | 1.00 | 43.27 | E |
| ATOM | 5425 | CD | ARG | E | 133 | 78.474 | 78.742 | -1.341 | 1.00 | 46.34 | E |
| ATOM | 5426 | NE | ARG | E | 133 | 79.096 | 80.006 | -1.738 | 1.00 | 49.86 | E |
| ATOM | 5427 | CZ | ARG | E | 133 | 78.441 | 81.058 | -2.226 | 1.00 | 51.63 | E |
| ATOM | 5428 | NH1 | ARG | E | 133 | 77.124 | 81.018 | -2.387 | 1.00 | 51.33 | E |
| ATOM | 5429 | NH2 | ARG | E | 133 | 79.111 | 82.155 | -2.562 | 1.00 | 52.46 | E |
| ATOM | 5430 | C | ARG | E | 133 | 75.343 | 78.204 | 1.792 | 1.00 | 38.70 | E |
| ATOM | 5431 | O | ARG | E | 133 | 74.569 | 78.154 | 0.835 | 1.00 | 38.81 | E |
| ATOM | 5432 | N | ASN | E | 134 | 75.119 | 78.940 | 2.872 | 1.00 | 39.37 | E |
| ATOM | 5433 | CA | ASN | E | 134 | 73.941 | 79.787 | 2.984 | 1.00 | 42.21 | E |
| ATOM | 5434 | CB | ASN | E | 134 | 74.040 | 80.952 | 1.988 | 1.00 | 40.37 | E |
| ATOM | 5435 | CG | ASN | E | 134 | 75.383 | 81.667 | 2.051 | 1.00 | 39.50 | E |
| ATOM | 5436 | OD1 | ASN | E | 134 | 75.796 | 82.151 | 3.104 | 1.00 | 35.36 | E |
| ATOM | 5437 | ND2 | ASN | E | 134 | 76.071 | 81.733 | 0.917 | 1.00 | 39.94 | E |
| ATOM | 5438 | C | ASN | E | 134 | 72.652 | 79.000 | 2.734 | 1.00 | 43.61 | E |
| ATOM | 5439 | O | ASN | E | 134 | 71.899 | 79.306 | 1.809 | 1.00 | 45.62 | E |
| ATOM | 5440 | N | ASP | E | 135 | 72.403 | 77.983 | 3.550 | 1.00 | 45.40 | E |
| ATOM | 5441 | CA | ASP | E | 135 | 71.189 | 77.178 | 3.413 | 1.00 | 47.16 | E |
| ATOM | 5442 | C | ASP | E | 135 | 71.147 | 76.279 | 2.173 | 1.00 | 48.15 | E |
| ATOM | 5443 | O | ASP | E | 135 | 70.205 | 75.504 | 1.996 | 1.00 | 49.25 | E |
| ATOM | 5444 | N | GLN | E | 136 | 72.158 | 76.387 | 1.316 | 1.00 | 48.16 | E |
| ATOM | 5445 | CA | GLN | E | 136 | 72.226 | 75.561 | 0.113 | 1.00 | 47.50 | E |
| ATOM | 5446 | C | GLN | E | 136 | 73.254 | 74.445 | 0.313 | 1.00 | 47.38 | E |
| ATOM | 5447 | O | GLN | E | 136 | 74.418 | 74.711 | 0.627 | 1.00 | 46.25 | E |
| ATOM | 5448 | N | GLU | E | 137 | 72.829 | 73.197 | 0.139 | 1.00 | 47.09 | E |
| ATOM | 5449 | CA | GLU | E | 137 | 73.749 | 72.079 | 0.308 | 1.00 | 47.41 | E |
| ATOM | 5450 | CB | GLU | E | 137 | 72.992 | 70.752 | 0.406 | 1.00 | 47.53 | E |
| ATOM | 5451 | CG | GLU | E | 137 | 73.921 | 69.570 | 0.653 | 1.00 | 49.67 | E |
| ATOM | 5452 | CD | GLU | E | 137 | 73.210 | 68.334 | 1.166 | 1.00 | 51.28 | E |
| ATOM | 5453 | OE1 | GLU | E | 137 | 73.911 | 67.336 | 1.432 | 1.00 | 52.31 | E |
| ATOM | 5454 | OE2 | GLU | E | 137 | 71.965 | 68.352 | 1.306 | 1.00 | 51.54 | E |
| ATOM | 5455 | C | GLU | E | 137 | 74.755 | 72.016 | -0.833 | 1.00 | 47.37 | E |
| ATOM | 5456 | O | GLU | E | 137 | 74.397 | 72.163 | -2.000 | 1.00 | 47.51 | E |
| ATOM | 5457 | N | GLU | E | 138 | 76.018 | 71.809 | -0.477 | 1.00 | 47.53 | E |
| ATOM | 5458 | CA | GLU | E | 138 | 77.104 | 71.724 | -1.444 | 1.00 | 48.48 | E |
| ATOM | 5459 | CB | GLU | E | 138 | 78.266 | 72.617 | -1.011 | 1.00 | 49.89 | E |
| ATOM | 5460 | CG | GLU | E | 138 | 77.949 | 74.096 | -0.973 | 1.00 | 54.83 | E |
| ATOM | 5461 | CD | GLU | E | 138 | 77.911 | 74.720 | -2.354 | 1.00 | 57.91 | E |
| ATOM | 5462 | OE1 | GLU | E | 138 | 78.953 | 74.686 | -3.044 | 1.00 | 59.04 | E |
| ATOM | 5463 | OE2 | GLU | E | 138 | 76.846 | 75.247 | -2.748 | 1.00 | 58.96 | E |
| ATOM | 5464 | C | GLU | E | 138 | 77.593 | 70.284 | -1.532 | 1.00 | 48.42 | E |
| ATOM | 5465 | O | GLU | E | 138 | 77.898 | 69.665 | -0.513 | 1.00 | 48.62 | E |
| ATOM | 5466 | N | THR | E | 139 | 77.665 | 69.754 | -2.748 | 1.00 | 47.87 | E |
| ATOM | 5467 | CA | THR | E | 139 | 78.135 | 68.387 | -2.959 | 1.00 | 48.16 | E |
| ATOM | 5468 | CB | THR | E | 139 | 77.027 | 67.498 | -3.556 | 1.00 | 49.05 | E |
| ATOM | 5469 | OG1 | THR | E | 139 | 76.464 | 68.140 | -4.710 | 1.00 | 51.25 | E |
| ATOM | 5470 | CG2 | THR | E | 139 | 75.938 | 67.249 | -2.525 | 1.00 | 48.03 | E |
| ATOM | 5471 | C | THR | E | 139 | 79.339 | 68.401 | -3.895 | 1.00 | 46.96 | E |

| ATOM | 5472 | O   | THR | E | 139 | 80.245 | 67.574 | -3.779 | 1.00 | 46.46 | E |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 5473 | N   | ALA | E | 140 | 79.339 | 69.346 | -4.827 | 1.00 | 46.59 | E |
| ATOM | 5474 | CA  | ALA | E | 140 | 80.446 | 69.488 | -5.761 | 1.00 | 45.07 | E |
| ATOM | 5475 | CB  | ALA | E | 140 | 79.997 | 70.244 | -7.008 | 1.00 | 44.64 | E |
| ATOM | 5476 | C   | ALA | E | 140 | 81.518 | 70.276 | -5.019 | 1.00 | 43.57 | E |
| ATOM | 5477 | O   | ALA | E | 140 | 81.224 | 71.293 | -4.386 | 1.00 | 43.33 | E |
| ATOM | 5478 | N   | GLY | E | 141 | 82.756 | 69.805 | -5.091 | 1.00 | 41.31 | E |
| ATOM | 5479 | CA  | GLY | E | 141 | 83.833 | 70.485 | -4.398 | 1.00 | 38.27 | E |
| ATOM | 5480 | C   | GLY | E | 141 | 84.053 | 69.854 | -3.034 | 1.00 | 36.91 | E |
| ATOM | 5481 | O   | GLY | E | 141 | 84.930 | 70.264 | -2.272 | 1.00 | 37.78 | E |
| ATOM | 5482 | N   | VAL | E | 142 | 83.245 | 68.849 | -2.722 | 1.00 | 33.36 | E |
| ATOM | 5483 | CA  | VAL | E | 142 | 83.363 | 68.164 | -1.449 | 1.00 | 32.16 | E |
| ATOM | 5484 | CB  | VAL | E | 142 | 81.978 | 67.844 | -0.847 | 1.00 | 31.40 | E |
| ATOM | 5485 | CG1 | VAL | E | 142 | 82.140 | 66.995 |  0.407 | 1.00 | 28.96 | E |
| ATOM | 5486 | CG2 | VAL | E | 142 | 81.245 | 69.134 | -0.516 | 1.00 | 33.20 | E |
| ATOM | 5487 | C   | VAL | E | 142 | 84.140 | 66.859 | -1.576 | 1.00 | 31.49 | E |
| ATOM | 5488 | O   | VAL | E | 142 | 83.862 | 66.032 | -2.450 | 1.00 | 31.67 | E |
| ATOM | 5489 | N   | VAL | E | 143 | 85.118 | 66.684 | -0.696 | 1.00 | 30.51 | E |
| ATOM | 5490 | CA  | VAL | E | 143 | 85.922 | 65.473 | -0.675 | 1.00 | 30.35 | E |
| ATOM | 5491 | CB  | VAL | E | 143 | 87.367 | 65.731 | -1.161 | 1.00 | 30.33 | E |
| ATOM | 5492 | CG1 | VAL | E | 143 | 88.096 | 64.408 | -1.348 | 1.00 | 32.44 | E |
| ATOM | 5493 | CG2 | VAL | E | 143 | 87.347 | 66.503 | -2.460 | 1.00 | 33.96 | E |
| ATOM | 5494 | C   | VAL | E | 143 | 85.966 | 64.973 |  0.767 | 1.00 | 29.68 | E |
| ATOM | 5495 | O   | VAL | E | 143 | 86.242 | 65.733 |  1.695 | 1.00 | 29.63 | E |
| ATOM | 5496 | N   | SER | E | 144 | 85.696 | 63.689 |  0.946 | 1.00 | 28.32 | E |
| ATOM | 5497 | CA  | SER | E | 144 | 85.703 | 63.090 |  2.268 | 1.00 | 25.38 | E |
| ATOM | 5498 | CB  | SER | E | 144 | 84.295 | 62.613 |  2.622 | 1.00 | 26.70 | E |
| ATOM | 5499 | OG  | SER | E | 144 | 84.300 | 61.845 |  3.807 | 1.00 | 28.37 | E |
| ATOM | 5500 | C   | SER | E | 144 | 86.663 | 61.916 |  2.361 | 1.00 | 24.56 | E |
| ATOM | 5501 | O   | SER | E | 144 | 86.824 | 61.148 |  1.412 | 1.00 | 23.42 | E |
| ATOM | 5502 | N   | THR | E | 145 | 87.320 | 61.790 |  3.506 | 1.00 | 24.40 | E |
| ATOM | 5503 | CA  | THR | E | 145 | 88.218 | 60.666 |  3.726 | 1.00 | 24.38 | E |
| ATOM | 5504 | CB  | THR | E | 145 | 89.103 | 60.849 |  4.983 | 1.00 | 24.55 | E |
| ATOM | 5505 | OG1 | THR | E | 145 | 88.273 | 60.815 |  6.155 | 1.00 | 21.59 | E |
| ATOM | 5506 | CG2 | THR | E | 145 | 89.858 | 62.162 |  4.935 | 1.00 | 24.64 | E |
| ATOM | 5507 | C   | THR | E | 145 | 87.256 | 59.539 |  4.055 | 1.00 | 23.78 | E |
| ATOM | 5508 | O   | THR | E | 145 | 86.064 | 59.766 |  4.242 | 1.00 | 23.97 | E |
| ATOM | 5509 | N   | PRO | E | 146 | 87.745 | 58.300 |  4.099 | 1.00 | 25.25 | E |
| ATOM | 5510 | CD  | PRO | E | 146 | 88.993 | 57.713 |  3.585 | 1.00 | 25.42 | E |
| ATOM | 5511 | CA  | PRO | E | 146 | 86.770 | 57.264 |  4.447 | 1.00 | 25.00 | E |
| ATOM | 5512 | CB  | PRO | E | 146 | 87.439 | 55.983 |  3.951 | 1.00 | 26.60 | E |
| ATOM | 5513 | CG  | PRO | E | 146 | 88.905 | 56.293 |  4.094 | 1.00 | 27.24 | E |
| ATOM | 5514 | C   | PRO | E | 146 | 86.597 | 57.284 |  5.976 | 1.00 | 23.26 | E |
| ATOM | 5515 | O   | PRO | E | 146 | 87.286 | 58.030 |  6.672 | 1.00 | 21.73 | E |
| ATOM | 5516 | N   | LEU | E | 147 | 85.669 | 56.492 |  6.495 | 1.00 | 23.85 | E |
| ATOM | 5517 | CA  | LEU | E | 147 | 85.476 | 56.419 |  7.936 | 1.00 | 23.63 | E |
| ATOM | 5518 | CB  | LEU | E | 147 | 84.355 | 55.428 |  8.260 | 1.00 | 25.11 | E |
| ATOM | 5519 | CG  | LEU | E | 147 | 83.976 | 55.241 |  9.731 | 1.00 | 28.28 | E |
| ATOM | 5520 | CD1 | LEU | E | 147 | 83.392 | 56.530 | 10.270 | 1.00 | 29.44 | E |
| ATOM | 5521 | CD2 | LEU | E | 147 | 82.965 | 54.116 |  9.867 | 1.00 | 28.72 | E |
| ATOM | 5522 | C   | LEU | E | 147 | 86.812 | 55.915 |  8.503 | 1.00 | 22.77 | E |
| ATOM | 5523 | O   | LEU | E | 147 | 87.366 | 54.944 |  8.003 | 1.00 | 23.04 | E |
| ATOM | 5524 | N   | ILE | E | 148 | 87.337 | 56.574 |  9.530 | 1.00 | 21.06 | E |
| ATOM | 5525 | CA  | ILE | E | 148 | 88.614 | 56.156 | 10.102 | 1.00 | 19.40 | E |
| ATOM | 5526 | CB  | ILE | E | 148 | 89.588 | 57.355 | 10.200 | 1.00 | 20.05 | E |
| ATOM | 5527 | CG2 | ILE | E | 148 | 90.903 | 56.922 | 10.835 | 1.00 | 19.93 | E |
| ATOM | 5528 | CG1 | ILE | E | 148 | 89.854 | 57.918 |  8.803 | 1.00 | 17.58 | E |
| ATOM | 5529 | CD1 | ILE | E | 148 | 90.594 | 59.225 |  8.821 | 1.00 | 20.23 | E |
| ATOM | 5530 | C   | ILE | E | 148 | 88.449 | 55.534 | 11.489 | 1.00 | 17.19 | E |
| ATOM | 5531 | O   | ILE | E | 148 | 87.820 | 56.118 | 12.360 | 1.00 | 15.81 | E |
| ATOM | 5532 | N   | ARG | E | 149 | 89.015 | 54.344 | 11.677 | 1.00 | 15.23 | E |
| ATOM | 5533 | CA  | ARG | E | 149 | 88.948 | 53.638 | 12.956 | 1.00 | 16.42 | E |
| ATOM | 5534 | CB  | ARG | E | 149 | 88.906 | 52.128 | 12.724 | 1.00 | 20.12 | E |
| ATOM | 5535 | CG  | ARG | E | 149 | 88.903 | 51.289 | 14.000 | 1.00 | 21.32 | E |
| ATOM | 5536 | CD  | ARG | E | 149 | 88.963 | 49.802 | 13.649 | 1.00 | 22.44 | E |
| ATOM | 5537 | NE  | ARG | E | 149 | 87.825 | 49.382 | 12.830 | 1.00 | 22.55 | E |
| ATOM | 5538 | CZ  | ARG | E | 149 | 86.623 | 49.084 | 13.313 | 1.00 | 22.89 | E |
| ATOM | 5539 | NH1 | ARG | E | 149 | 85.650 | 48.718 | 12.490 | 1.00 | 24.25 | E |
| ATOM | 5540 | NH2 | ARG | E | 149 | 86.398 | 49.139 | 14.619 | 1.00 | 23.36 | E |
| ATOM | 5541 | C   | ARG | E | 149 | 90.174 | 53.983 | 13.786 | 1.00 | 16.33 | E |
| ATOM | 5542 | O   | ARG | E | 149 | 91.305 | 53.734 | 13.363 | 1.00 | 16.45 | E |
| ATOM | 5543 | N   | ASN | E | 150 | 89.953 | 54.558 | 14.963 | 1.00 | 15.72 | E |
| ATOM | 5544 | CA  | ASN | E | 150 | 91.061 | 54.948 | 15.825 | 1.00 | 15.93 | E |
| ATOM | 5545 | CB  | ASN | E | 150 | 90.662 | 56.125 | 16.740 | 1.00 | 13.37 | E |

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| ATOM | 5546 | CG | ASN | E | 150 | 90.278 | 57.383 | 15.955 | 1.00 | 15.55 | E |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 5547 | OD1 | ASN | E | 150 | 90.922 | 57.739 | 14.955 | 1.00 | 14.20 | E |
| ATOM | 5548 | ND2 | ASN | E | 150 | 89.233 | 58.068 | 16.414 | 1.00 | 15.61 | E |
| ATOM | 5549 | C | ASN | E | 150 | 91.576 | 53.786 | 16.670 | 1.00 | 16.79 | E |
| ATOM | 5550 | O | ASN | E | 150 | 92.694 | 53.838 | 17.180 | 1.00 | 18.80 | E |
| ATOM | 5551 | N | GLY | E | 151 | 90.764 | 52.745 | 16.813 | 1.00 | 16.63 | E |
| ATOM | 5552 | CA | GLY | E | 151 | 91.164 | 51.587 | 17.593 | 1.00 | 18.68 | E |
| ATOM | 5553 | C | GLY | E | 151 | 90.879 | 51.684 | 19.080 | 1.00 | 20.19 | E |
| ATOM | 5554 | O | GLY | E | 151 | 91.087 | 50.725 | 19.818 | 1.00 | 21.39 | E |
| ATOM | 5555 | N | ASP | E | 152 | 90.409 | 52.836 | 19.539 | 1.00 | 19.57 | E |
| ATOM | 5556 | CA | ASP | E | 152 | 90.108 | 52.986 | 20.954 | 1.00 | 19.09 | E |
| ATOM | 5557 | CB | ASP | E | 152 | 90.865 | 54.177 | 21.531 | 1.00 | 18.53 | E |
| ATOM | 5558 | CG | ASP | E | 152 | 90.498 | 55.481 | 20.856 | 1.00 | 21.27 | E |
| ATOM | 5559 | OD1 | ASP | E | 152 | 89.736 | 55.453 | 19.864 | 1.00 | 20.11 | E |
| ATOM | 5560 | OD2 | ASP | E | 152 | 90.984 | 56.531 | 21.321 | 1.00 | 22.57 | E |
| ATOM | 5561 | C | ASP | E | 152 | 88.605 | 53.156 | 21.182 | 1.00 | 19.23 | E |
| ATOM | 5562 | O | ASP | E | 152 | 88.177 | 53.840 | 22.113 | 1.00 | 17.78 | E |
| ATOM | 5563 | N | TRP | E | 153 | 87.816 | 52.522 | 20.318 | 1.00 | 18.88 | E |
| ATOM | 5564 | CA | TRP | E | 153 | 86.356 | 52.566 | 20.391 | 1.00 | 18.61 | E |
| ATOM | 5565 | CB | TRP | E | 153 | 85.862 | 52.162 | 21.788 | 1.00 | 17.06 | E |
| ATOM | 5566 | CG | TRP | E | 153 | 86.084 | 50.690 | 22.085 | 1.00 | 17.90 | E |
| ATOM | 5567 | CD2 | TRP | E | 153 | 85.165 | 49.612 | 21.830 | 1.00 | 18.84 | E |
| ATOM | 5568 | CE2 | TRP | E | 153 | 85.804 | 48.414 | 22.222 | 1.00 | 16.88 | E |
| ATOM | 5569 | CE3 | TRP | E | 153 | 83.862 | 49.544 | 21.308 | 1.00 | 18.29 | E |
| ATOM | 5570 | CD1 | TRP | E | 153 | 87.209 | 50.114 | 22.604 | 1.00 | 16.70 | E |
| ATOM | 5571 | NE1 | TRP | E | 153 | 87.049 | 48.747 | 22.688 | 1.00 | 17.49 | E |
| ATOM | 5572 | CZ2 | TRP | E | 153 | 85.189 | 47.164 | 22.109 | 1.00 | 16.54 | E |
| ATOM | 5573 | CZ3 | TRP | E | 153 | 83.250 | 48.303 | 21.196 | 1.00 | 17.19 | E |
| ATOM | 5574 | CH2 | TRP | E | 153 | 83.917 | 47.129 | 21.597 | 1.00 | 17.24 | E |
| ATOM | 5575 | C | TRP | E | 153 | 85.732 | 53.887 | 19.975 | 1.00 | 18.97 | E |
| ATOM | 5576 | O | TRP | E | 153 | 84.696 | 54.300 | 20.508 | 1.00 | 18.70 | E |
| ATOM | 5577 | N | THR | E | 154 | 86.378 | 54.546 | 19.016 | 1.00 | 19.20 | E |
| ATOM | 5578 | CA | THR | E | 154 | 85.876 | 55.794 | 18.444 | 1.00 | 19.92 | E |
| ATOM | 5579 | CB | THR | E | 154 | 86.442 | 57.072 | 19.129 | 1.00 | 21.42 | E |
| ATOM | 5580 | OG1 | THR | E | 154 | 87.865 | 57.129 | 18.958 | 1.00 | 19.26 | E |
| ATOM | 5581 | CG2 | THR | E | 154 | 86.085 | 57.096 | 20.599 | 1.00 | 22.17 | E |
| ATOM | 5582 | C | THR | E | 154 | 86.314 | 55.835 | 16.992 | 1.00 | 18.66 | E |
| ATOM | 5583 | O | THR | E | 154 | 87.270 | 55.156 | 16.603 | 1.00 | 19.45 | E |
| ATOM | 5584 | N | PHE | E | 155 | 85.609 | 56.626 | 16.193 | 1.00 | 18.54 | E |
| ATOM | 5585 | CA | PHE | E | 155 | 85.940 | 56.784 | 14.779 | 1.00 | 19.04 | E |
| ATOM | 5586 | CB | PHE | E | 155 | 84.821 | 56.252 | 13.882 | 1.00 | 20.71 | E |
| ATOM | 5587 | CG | PHE | E | 155 | 84.524 | 54.794 | 14.060 | 1.00 | 23.03 | E |
| ATOM | 5588 | CD1 | PHE | E | 155 | 83.492 | 54.375 | 14.898 | 1.00 | 23.94 | E |
| ATOM | 5589 | CD2 | PHE | E | 155 | 85.255 | 53.837 | 13.365 | 1.00 | 23.32 | E |
| ATOM | 5590 | CE1 | PHE | E | 155 | 83.189 | 53.017 | 15.037 | 1.00 | 23.82 | E |
| ATOM | 5591 | CE2 | PHE | E | 155 | 84.962 | 52.476 | 13.497 | 1.00 | 24.46 | E |
| ATOM | 5592 | CZ | PHE | E | 155 | 83.930 | 52.068 | 14.333 | 1.00 | 24.51 | E |
| ATOM | 5593 | C | PHE | E | 155 | 86.109 | 58.265 | 14.459 | 1.00 | 19.30 | E |
| ATOM | 5594 | O | PHE | E | 155 | 85.791 | 59.134 | 15.275 | 1.00 | 19.12 | E |
| ATOM | 5595 | N | GLN | E | 156 | 86.613 | 58.550 | 13.265 | 1.00 | 17.46 | E |
| ATOM | 5596 | CA | GLN | E | 156 | 86.748 | 59.924 | 12.824 | 1.00 | 17.87 | E |
| ATOM | 5597 | CB | GLN | E | 156 | 88.081 | 60.546 | 13.264 | 1.00 | 19.74 | E |
| ATOM | 5598 | CG | GLN | E | 156 | 89.330 | 59.948 | 12.640 | 1.00 | 19.80 | E |
| ATOM | 5599 | CD | GLN | E | 156 | 90.551 | 60.785 | 12.950 | 1.00 | 21.46 | E |
| ATOM | 5600 | OE1 | GLN | E | 156 | 90.660 | 61.928 | 12.503 | 1.00 | 21.30 | E |
| ATOM | 5601 | NE2 | GLN | E | 156 | 91.469 | 60.230 | 13.734 | 1.00 | 21.38 | E |
| ATOM | 5602 | C | GLN | E | 156 | 86.629 | 59.989 | 11.316 | 1.00 | 17.47 | E |
| ATOM | 5603 | O | GLN | E | 156 | 86.856 | 58.999 | 10.616 | 1.00 | 17.25 | E |
| ATOM | 5604 | N | ILE | E | 157 | 86.252 | 61.159 | 10.823 | 1.00 | 17.46 | E |
| ATOM | 5605 | CA | ILE | E | 157 | 86.128 | 61.363 | 9.397 | 1.00 | 18.92 | E |
| ATOM | 5606 | CB | ILE | E | 157 | 84.746 | 60.922 | 8.898 | 1.00 | 19.57 | E |
| ATOM | 5607 | CG2 | ILE | E | 157 | 83.659 | 61.774 | 9.545 | 1.00 | 15.09 | E |
| ATOM | 5608 | CG1 | ILE | E | 157 | 84.704 | 60.994 | 7.369 | 1.00 | 21.06 | E |
| ATOM | 5609 | CD1 | ILE | E | 157 | 83.541 | 60.218 | 6.756 | 1.00 | 22.57 | E |
| ATOM | 5610 | C | ILE | E | 157 | 86.349 | 62.837 | 9.083 | 1.00 | 20.28 | E |
| ATOM | 5611 | O | ILE | E | 157 | 85.887 | 63.712 | 9.808 | 1.00 | 20.70 | E |
| ATOM | 5612 | N | LEU | E | 158 | 87.094 | 63.104 | 8.019 | 1.00 | 21.79 | E |
| ATOM | 5613 | CA | LEU | E | 158 | 87.363 | 64.470 | 7.601 | 1.00 | 23.40 | E |
| ATOM | 5614 | CB | LEU | E | 158 | 88.869 | 64.706 | 7.466 | 1.00 | 25.42 | E |
| ATOM | 5615 | CG | LEU | E | 158 | 89.621 | 65.141 | 8.731 | 1.00 | 29.38 | E |
| ATOM | 5616 | CD1 | LEU | E | 158 | 89.384 | 64.154 | 9.864 | 1.00 | 27.98 | E |
| ATOM | 5617 | CD2 | LEU | E | 158 | 91.118 | 65.263 | 8.412 | 1.00 | 30.79 | E |
| ATOM | 5618 | C | LEU | E | 158 | 86.664 | 64.738 | 6.271 | 1.00 | 23.62 | E |
| ATOM | 5619 | O | LEU | E | 158 | 86.938 | 64.081 | 5.264 | 1.00 | 22.86 | E |

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ATOM   5620  N    VAL E 159    85.747  65.702   6.290  1.00 22.98      E
ATOM   5621  CA   VAL E 159    84.990  66.087   5.112  1.00 21.37      E
ATOM   5622  CB   VAL E 159    83.476  66.104   5.417  1.00 20.53      E
ATOM   5623  CG1  VAL E 159    82.684  66.407   4.149  1.00 14.20      E
ATOM   5624  CG2  VAL E 159    83.058  64.756   6.002  1.00 15.86      E
ATOM   5625  C    VAL E 159    85.468  67.469   4.710  1.00 22.21      E
ATOM   5626  O    VAL E 159    85.253  68.444   5.423  1.00 22.87      E
ATOM   5627  N    MET E 160    86.116  67.539   3.555  1.00 25.37      E
ATOM   5628  CA   MET E 160    86.681  68.779   3.049  1.00 27.07      E
ATOM   5629  CB   MET E 160    88.088  68.494   2.533  1.00 29.57      E
ATOM   5630  CG   MET E 160    88.996  67.954   3.633  1.00 35.17      E
ATOM   5631  SD   MET E 160    90.519  67.185   3.065  1.00 41.54      E
ATOM   5632  CE   MET E 160    90.011  65.462   2.985  1.00 40.10      E
ATOM   5633  C    MET E 160    85.848  69.466   1.979  1.00 28.93      E
ATOM   5634  O    MET E 160    85.191  68.817   1.162  1.00 28.47      E
ATOM   5635  N    LEU E 161    85.875  70.793   1.997  1.00 29.41      E
ATOM   5636  CA   LEU E 161    85.123  71.574   1.031  1.00 31.54      E
ATOM   5637  CB   LEU E 161    83.931  72.258   1.708  1.00 30.26      E
ATOM   5638  CG   LEU E 161    83.183  73.297   0.860  1.00 30.70      E
ATOM   5639  CD1  LEU E 161    82.515  72.618  -0.332  1.00 29.72      E
ATOM   5640  CD2  LEU E 161    82.145  74.020   1.728  1.00 31.55      E
ATOM   5641  C    LEU E 161    85.990  72.625   0.363  1.00 32.10      E
ATOM   5642  O    LEU E 161    86.575  73.473   1.029  1.00 32.90      E
ATOM   5643  N    GLU E 162    86.063  72.549  -0.960  1.00 35.11      E
ATOM   5644  CA   GLU E 162    86.820  73.491  -1.771  1.00 38.40      E
ATOM   5645  CB   GLU E 162    87.191  72.838  -3.105  1.00 42.17      E
ATOM   5646  CG   GLU E 162    87.783  73.776  -4.148  1.00 48.21      E
ATOM   5647  CD   GLU E 162    89.099  74.381  -3.711  1.00 52.47      E
ATOM   5648  OE1  GLU E 162    90.006  73.611  -3.327  1.00 54.02      E
ATOM   5649  OE2  GLU E 162    89.228  75.627  -3.759  1.00 56.21      E
ATOM   5650  C    GLU E 162    85.892  74.673  -2.008  1.00 39.06      E
ATOM   5651  O    GLU E 162    84.750  74.490  -2.422  1.00 39.27      E
ATOM   5652  N    MET E 163    86.369  75.884  -1.747  1.00 40.73      E
ATOM   5653  CA   MET E 163    85.520  77.049  -1.938  1.00 43.18      E
ATOM   5654  CB   MET E 163    84.546  77.171  -0.761  1.00 45.15      E
ATOM   5655  CG   MET E 163    85.155  76.900   0.612  1.00 47.55      E
ATOM   5656  SD   MET E 163    86.318  78.152   1.185  1.00 52.18      E
ATOM   5657  CE   MET E 163    85.186  79.345   1.941  1.00 50.37      E
ATOM   5658  C    MET E 163    86.245  78.371  -2.151  1.00 43.77      E
ATOM   5659  O    MET E 163    87.458  78.477  -1.953  1.00 41.87      E
ATOM   5660  N    THR E 164    85.474  79.371  -2.571  1.00 45.83      E
ATOM   5661  CA   THR E 164    85.981  80.714  -2.827  1.00 49.20      E
ATOM   5662  CB   THR E 164    85.585  81.177  -4.241  1.00 50.11      E
ATOM   5663  OG1  THR E 164    86.036  80.208  -5.199  1.00 49.28      E
ATOM   5664  CG2  THR E 164    86.204  82.535  -4.559  1.00 50.19      E
ATOM   5665  C    THR E 164    85.371  81.652  -1.785  1.00 51.14      E
ATOM   5666  O    THR E 164    84.169  81.916  -1.802  1.00 50.64      E
ATOM   5667  N    PRO E 165    86.198  82.170  -0.864  1.00 53.75      E
ATOM   5668  CD   PRO E 165    87.667  82.057  -0.818  1.00 54.65      E
ATOM   5669  CA   PRO E 165    85.719  83.072   0.185  1.00 56.16      E
ATOM   5670  CB   PRO E 165    86.965  83.299   1.036  1.00 55.47      E
ATOM   5671  CG   PRO E 165    88.057  83.262   0.019  1.00 55.93      E
ATOM   5672  C    PRO E 165    85.098  84.381  -0.291  1.00 58.83      E
ATOM   5673  O    PRO E 165    85.673  85.100  -1.112  1.00 58.35      E
ATOM   5674  N    GLN E 166    83.912  84.666   0.239  1.00 61.77      E
ATOM   5675  CA   GLN E 166    83.173  85.885  -0.065  1.00 63.96      E
ATOM   5676  CB   GLN E 166    82.103  85.616  -1.123  1.00 64.28      E
ATOM   5677  CG   GLN E 166    82.662  85.236  -2.481  1.00 66.42      E
ATOM   5678  CD   GLN E 166    81.643  85.392  -3.596  1.00 67.38      E
ATOM   5679  OE1  GLN E 166    81.937  85.124  -4.761  1.00 68.28      E
ATOM   5680  NE2  GLN E 166    80.437  85.832  -3.244  1.00 66.50      E
ATOM   5681  C    GLN E 166    82.521  86.396   1.223  1.00 65.40      E
ATOM   5682  O    GLN E 166    81.974  85.614   2.007  1.00 65.65      E
ATOM   5683  N    ARG E 167    82.589  87.707   1.444  1.00 65.80      E
ATOM   5684  CA   ARG E 167    82.017  88.302   2.647  1.00 65.27      E
ATOM   5685  CB   ARG E 167    82.353  89.795   2.706  1.00 67.87      E
ATOM   5686  CG   ARG E 167    82.221  90.423   4.095  1.00 70.91      E
ATOM   5687  CD   ARG E 167    83.216  89.813   5.085  1.00 73.36      E
ATOM   5688  NE   ARG E 167    83.244  90.532   6.359  1.00 75.19      E
ATOM   5689  CZ   ARG E 167    84.012  90.199   7.394  1.00 75.48      E
ATOM   5690  NH1  ARG E 167    84.824  89.151   7.318  1.00 75.50      E
ATOM   5691  NH2  ARG E 167    83.968  90.916   8.509  1.00 75.83      E
ATOM   5692  C    ARG E 167    80.504  88.100   2.684  1.00 63.81      E
ATOM   5693  O    ARG E 167    79.816  88.254   1.672  1.00 62.94      E
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ATOM   5694  N   GLY E 168      79.991  87.751   3.860  1.00 61.88           E
ATOM   5695  CA  GLY E 168      78.567  87.519   4.004  1.00 58.78           E
ATOM   5696  C   GLY E 168      78.243  86.036   3.959  1.00 57.24           E
ATOM   5697  O   GLY E 168      77.262  85.594   4.558  1.00 57.26           E
ATOM   5698  N   ASP E 169      79.066  85.263   3.249  1.00 54.67           E
ATOM   5699  CA  ASP E 169      78.849  83.823   3.140  1.00 52.07           E
ATOM   5700  CB  ASP E 169      79.799  83.186   2.116  1.00 52.03           E
ATOM   5701  CG  ASP E 169      79.329  83.359   0.683  1.00 52.57           E
ATOM   5702  OD1 ASP E 169      78.105  83.453   0.457  1.00 51.86           E
ATOM   5703  OD2 ASP E 169      80.188  83.376  -0.223  1.00 52.34           E
ATOM   5704  C   ASP E 169      79.027  83.096   4.463  1.00 49.54           E
ATOM   5705  O   ASP E 169      79.993  83.322   5.196  1.00 49.84           E
ATOM   5706  N   VAL E 170      78.082  82.214   4.758  1.00 46.54           E
ATOM   5707  CA  VAL E 170      78.136  81.418   5.970  1.00 43.15           E
ATOM   5708  CB  VAL E 170      76.903  81.669   6.871  1.00 42.70           E
ATOM   5709  CG1 VAL E 170      76.997  80.819   8.138  1.00 41.36           E
ATOM   5710  CG2 VAL E 170      76.814  83.146   7.227  1.00 41.14           E
ATOM   5711  C   VAL E 170      78.172  79.948   5.555  1.00 41.66           E
ATOM   5712  O   VAL E 170      77.216  79.432   4.972  1.00 40.25           E
ATOM   5713  N   TYR E 171      79.289  79.287   5.833  1.00 39.16           E
ATOM   5714  CA  TYR E 171      79.438  77.877   5.502  1.00 38.16           E
ATOM   5715  CB  TYR E 171      80.836  77.617   4.953  1.00 38.66           E
ATOM   5716  CG  TYR E 171      81.035  78.237   3.598  1.00 38.98           E
ATOM   5717  CD1 TYR E 171      80.740  77.522   2.440  1.00 38.79           E
ATOM   5718  CE1 TYR E 171      80.852  78.105   1.186  1.00 40.42           E
ATOM   5719  CD2 TYR E 171      81.451  79.561   3.471  1.00 38.62           E
ATOM   5720  CE2 TYR E 171      81.565  80.160   2.219  1.00 40.32           E
ATOM   5721  CZ  TYR E 171      81.262  79.424   1.079  1.00 41.26           E
ATOM   5722  OH  TYR E 171      81.350  80.004  -0.166  1.00 42.98           E
ATOM   5723  C   TYR E 171      79.206  77.076   6.764  1.00 37.15           E
ATOM   5724  O   TYR E 171      79.755  77.398   7.813  1.00 37.94           E
ATOM   5725  N   THR E 172      78.384  76.037   6.672  1.00 35.12           E
ATOM   5726  CA  THR E 172      78.091  75.229   7.842  1.00 34.42           E
ATOM   5727  CB  THR E 172      76.654  75.496   8.367  1.00 35.21           E
ATOM   5728  OG1 THR E 172      76.184  74.351   9.094  1.00 35.96           E
ATOM   5729  CG2 THR E 172      75.706  75.790   7.226  1.00 38.35           E
ATOM   5730  C   THR E 172      78.263  73.734   7.638  1.00 32.90           E
ATOM   5731  O   THR E 172      77.875  73.188   6.604  1.00 31.57           E
ATOM   5732  N   CYS E 173      78.858  73.090   8.643  1.00 30.59           E
ATOM   5733  CA  CYS E 173      79.078  71.646   8.640  1.00 29.35           E
ATOM   5734  C   CYS E 173      77.923  71.058   9.454  1.00 29.72           E
ATOM   5735  O   CYS E 173      77.771  71.337  10.645  1.00 28.89           E
ATOM   5736  CB  CYS E 173      80.424  71.299   9.287  1.00 27.53           E
ATOM   5737  SG  CYS E 173      80.875  69.541   9.133  1.00 27.81           E
ATOM   5738  N   HIS E 174      77.109  70.251   8.788  1.00 28.95           E
ATOM   5739  CA  HIS E 174      75.925  69.642   9.381  1.00 28.54           E
ATOM   5740  CB  HIS E 174      74.770  69.881   8.399  1.00 29.66           E
ATOM   5741  CG  HIS E 174      73.457  69.311   8.823  1.00 30.98           E
ATOM   5742  CD2 HIS E 174      72.367  69.899   9.369  1.00 31.91           E
ATOM   5743  ND1 HIS E 174      73.124  67.988   8.630  1.00 31.68           E
ATOM   5744  CE1 HIS E 174      71.883  67.785   9.034  1.00 33.26           E
ATOM   5745  NE2 HIS E 174      71.401  68.929   9.487  1.00 34.66           E
ATOM   5746  C   HIS E 174      76.173  68.151   9.650  1.00 27.83           E
ATOM   5747  O   HIS E 174      76.438  67.375   8.728  1.00 27.35           E
ATOM   5748  N   VAL E 175      76.085  67.753  10.917  1.00 26.27           E
ATOM   5749  CA  VAL E 175      76.349  66.365  11.284  1.00 26.34           E
ATOM   5750  CB  VAL E 175      77.584  66.281  12.215  1.00 23.90           E
ATOM   5751  CG1 VAL E 175      77.807  64.850  12.663  1.00 19.67           E
ATOM   5752  CG2 VAL E 175      78.818  66.813  11.491  1.00 19.93           E
ATOM   5753  C   VAL E 175      75.199  65.603  11.938  1.00 27.67           E
ATOM   5754  O   VAL E 175      74.587  66.064  12.904  1.00 26.77           E
ATOM   5755  N   GLU E 176      74.917  64.423  11.399  1.00 29.83           E
ATOM   5756  CA  GLU E 176      73.864  63.564  11.929  1.00 32.99           E
ATOM   5757  CB  GLU E 176      72.842  63.231  10.839  1.00 34.86           E
ATOM   5758  CG  GLU E 176      72.076  64.441  10.319  1.00 40.13           E
ATOM   5759  CD  GLU E 176      71.204  64.107   9.124  1.00 44.38           E
ATOM   5760  OE1 GLU E 176      70.292  63.265   9.269  1.00 46.31           E
ATOM   5761  OE2 GLU E 176      71.433  64.682   8.037  1.00 47.49           E
ATOM   5762  C   GLU E 176      74.526  62.289  12.445  1.00 32.24           E
ATOM   5763  O   GLU E 176      75.296  61.646  11.734  1.00 32.81           E
ATOM   5764  N   HIS E 177      74.220  61.934  13.686  1.00 31.66           E
ATOM   5765  CA  HIS E 177      74.803  60.761  14.311  1.00 30.50           E
ATOM   5766  CB  HIS E 177      76.147  61.161  14.927  1.00 29.59           E
ATOM   5767  CG  HIS E 177      76.871  60.034  15.582  1.00 28.23           E
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ATOM   5768  CD2 HIS E 177    77.752  59.134  15.086  1.00 28.22      E
ATOM   5769  ND1 HIS E 177    76.679  59.698  16.903  1.00 27.71      E
ATOM   5770  CE1 HIS E 177    77.410  58.636  17.194  1.00 29.83      E
ATOM   5771  NE2 HIS E 177    78.070  58.274  16.108  1.00 29.78      E
ATOM   5772  C   HIS E 177    73.854  60.195  15.373  1.00 30.09      E
ATOM   5773  O   HIS E 177    73.189  60.942  16.083  1.00 29.91      E
ATOM   5774  N   PRO E 178    73.781  58.862  15.496  1.00 31.45      E
ATOM   5775  CD  PRO E 178    74.485  57.842  14.697  1.00 31.00      E
ATOM   5776  CA  PRO E 178    72.898  58.226  16.481  1.00 31.44      E
ATOM   5777  CB  PRO E 178    73.370  56.779  16.467  1.00 30.89      E
ATOM   5778  CG  PRO E 178    73.704  56.578  15.028  1.00 31.16      E
ATOM   5779  C   PRO E 178    72.896  58.826  17.893  1.00 31.78      E
ATOM   5780  O   PRO E 178    71.903  58.727  18.611  1.00 32.84      E
ATOM   5781  N   SER E 179    73.996  59.448  18.292  1.00 30.31      E
ATOM   5782  CA  SER E 179    74.087  60.039  19.624  1.00 30.84      E
ATOM   5783  CB  SER E 179    75.552  60.155  20.038  1.00 29.11      E
ATOM   5784  OG  SER E 179    76.240  61.049  19.176  1.00 24.79      E
ATOM   5785  C   SER E 179    73.452  61.424  19.717  1.00 32.75      E
ATOM   5786  O   SER E 179    73.330  61.982  20.804  1.00 32.78      E
ATOM   5787  N   LEU E 180    73.046  61.981  18.583  1.00 35.18      E
ATOM   5788  CA  LEU E 180    72.477  63.317  18.578  1.00 37.31      E
ATOM   5789  CB  LEU E 180    73.098  64.132  17.448  1.00 35.77      E
ATOM   5790  CG  LEU E 180    74.610  64.337  17.528  1.00 36.46      E
ATOM   5791  CD1 LEU E 180    75.097  65.018  16.259  1.00 35.16      E
ATOM   5792  CD2 LEU E 180    74.948  65.167  18.752  1.00 34.58      E
ATOM   5793  C   LEU E 180    70.967  63.405  18.463  1.00 40.35      E
ATOM   5794  O   LEU E 180    70.386  63.003  17.456  1.00 40.67      E
ATOM   5795  N   GLN E 181    70.338  63.943  19.503  1.00 42.97      E
ATOM   5796  CA  GLN E 181    68.895  64.141  19.504  1.00 45.09      E
ATOM   5797  CB  GLN E 181    68.466  64.877  20.776  1.00 46.73      E
ATOM   5798  CG  GLN E 181    69.471  65.931  21.235  1.00 49.84      E
ATOM   5799  CD  GLN E 181    68.898  66.904  22.256  1.00 52.17      E
ATOM   5800  OE1 GLN E 181    68.074  67.760  21.920  1.00 52.91      E
ATOM   5801  NE2 GLN E 181    69.329  66.774  23.510  1.00 51.73      E
ATOM   5802  C   GLN E 181    68.607  65.002  18.277  1.00 45.26      E
ATOM   5803  O   GLN E 181    67.660  64.752  17.530  1.00 46.25      E
ATOM   5804  N   SER E 182    69.448  66.013  18.078  1.00 44.33      E
ATOM   5805  CA  SER E 182    69.335  66.923  16.943  1.00 42.52      E
ATOM   5806  CB  SER E 182    68.819  68.291  17.401  1.00 43.41      E
ATOM   5807  OG  SER E 182    69.658  68.853  18.396  1.00 43.07      E
ATOM   5808  C   SER E 182    70.725  67.068  16.337  1.00 41.70      E
ATOM   5809  O   SER E 182    71.726  66.955  17.040  1.00 39.94      E
ATOM   5810  N   PRO E 183    70.805  67.330  15.023  1.00 41.57      E
ATOM   5811  CD  PRO E 183    69.680  67.554  14.098  1.00 41.72      E
ATOM   5812  CA  PRO E 183    72.087  67.485  14.326  1.00 40.68      E
ATOM   5813  CB  PRO E 183    71.669  67.638  12.865  1.00 40.95      E
ATOM   5814  CG  PRO E 183    70.344  68.309  12.965  1.00 42.76      E
ATOM   5815  C   PRO E 183    72.988  68.628  14.790  1.00 38.81      E
ATOM   5816  O   PRO E 183    72.520  69.709  15.142  1.00 39.64      E
ATOM   5817  N   ILE E 184    74.291  68.370  14.785  1.00 37.31      E
ATOM   5818  CA  ILE E 184    75.270  69.368  15.177  1.00 34.30      E
ATOM   5819  CB  ILE E 184    76.570  68.728  15.699  1.00 33.43      E
ATOM   5820  CG2 ILE E 184    77.671  69.779  15.766  1.00 32.87      E
ATOM   5821  CG1 ILE E 184    76.337  68.112  17.076  1.00 33.53      E
ATOM   5822  CD1 ILE E 184    77.530  67.339  17.604  1.00 33.29      E
ATOM   5823  C   ILE E 184    75.625  70.216  13.974  1.00 33.68      E
ATOM   5824  O   ILE E 184    75.851  69.704  12.882  1.00 33.87      E
ATOM   5825  N   THR E 185    75.676  71.521  14.181  1.00 34.19      E
ATOM   5826  CA  THR E 185    76.018  72.431  13.111  1.00 33.39      E
ATOM   5827  CB  THR E 185    74.792  73.230  12.637  1.00 33.77      E
ATOM   5828  OG1 THR E 185    74.211  73.918  13.751  1.00 33.46      E
ATOM   5829  CG2 THR E 185    73.758  72.297  12.016  1.00 33.35      E
ATOM   5830  C   THR E 185    77.081  73.396  13.590  1.00 33.01      E
ATOM   5831  O   THR E 185    76.990  73.966  14.679  1.00 33.25      E
ATOM   5832  N   VAL E 186    78.106  73.552  12.770  1.00 32.85      E
ATOM   5833  CA  VAL E 186    79.197  74.453  13.067  1.00 32.84      E
ATOM   5834  CB  VAL E 186    80.503  73.684  13.300  1.00 31.58      E
ATOM   5835  CG1 VAL E 186    81.629  74.651  13.611  1.00 30.07      E
ATOM   5836  CG2 VAL E 186    80.316  72.697  14.441  1.00 30.84      E
ATOM   5837  C   VAL E 186    79.329  75.317  11.836  1.00 34.14      E
ATOM   5838  O   VAL E 186    79.403  74.812  10.719  1.00 33.50      E
ATOM   5839  N   GLU E 187    79.329  76.626  12.029  1.00 38.05      E
ATOM   5840  CA  GLU E 187    79.453  77.522  10.898  1.00 40.60      E
ATOM   5841  CB  GLU E 187    78.358  78.592  10.934  1.00 43.36      E
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| ATOM | 5842 | CG  | GLU | E | 187 | 78.426 | 79.531 | 12.121 | 1.00 | 47.46 | E |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 5843 | CD  | GLU | E | 187 | 77.657 | 80.822 | 11.886 | 1.00 | 51.49 | E |
| ATOM | 5844 | OE1 | GLU | E | 187 | 76.452 | 80.752 | 11.551 | 1.00 | 52.89 | E |
| ATOM | 5845 | OE2 | GLU | E | 187 | 78.262 | 81.908 | 12.039 | 1.00 | 53.48 | E |
| ATOM | 5846 | C   | GLU | E | 187 | 80.819 | 78.182 | 10.877 | 1.00 | 40.49 | E |
| ATOM | 5847 | O   | GLU | E | 187 | 81.496 | 78.285 | 11.901 | 1.00 | 40.26 | E |
| ATOM | 5848 | N   | TRP | E | 188 | 81.221 | 78.610 | 9.688  | 1.00 | 41.52 | E |
| ATOM | 5849 | CA  | TRP | E | 188 | 82.492 | 79.284 | 9.488  | 1.00 | 43.59 | E |
| ATOM | 5850 | CB  | TRP | E | 188 | 83.498 | 78.337 | 8.834  | 1.00 | 41.24 | E |
| ATOM | 5851 | CG  | TRP | E | 188 | 84.852 | 78.942 | 8.675  | 1.00 | 41.34 | E |
| ATOM | 5852 | CD2 | TRP | E | 188 | 85.327 | 79.672 | 7.543  | 1.00 | 40.23 | E |
| ATOM | 5853 | CE2 | TRP | E | 188 | 86.642 | 80.090 | 7.838  | 1.00 | 41.87 | E |
| ATOM | 5854 | CE3 | TRP | E | 188 | 84.768 | 80.015 | 6.305  | 1.00 | 40.90 | E |
| ATOM | 5855 | CD1 | TRP | E | 188 | 85.867 | 78.945 | 9.588  | 1.00 | 41.88 | E |
| ATOM | 5856 | NE1 | TRP | E | 188 | 86.947 | 79.632 | 9.093  | 1.00 | 41.99 | E |
| ATOM | 5857 | CZ2 | TRP | E | 188 | 87.411 | 80.835 | 6.938  | 1.00 | 42.93 | E |
| ATOM | 5858 | CZ3 | TRP | E | 188 | 85.531 | 80.757 | 5.408  | 1.00 | 42.58 | E |
| ATOM | 5859 | CH2 | TRP | E | 188 | 86.839 | 81.159 | 5.731  | 1.00 | 43.65 | E |
| ATOM | 5860 | C   | TRP | E | 188 | 82.198 | 80.467 | 8.566  | 1.00 | 46.04 | E |
| ATOM | 5861 | O   | TRP | E | 188 | 81.335 | 80.374 | 7.688  | 1.00 | 45.30 | E |
| ATOM | 5862 | N   | ARG | E | 189 | 82.899 | 81.579 | 8.765  | 1.00 | 50.26 | E |
| ATOM | 5863 | CA  | ARG | E | 189 | 82.673 | 82.761 | 7.936  | 1.00 | 54.31 | E |
| ATOM | 5864 | CB  | ARG | E | 189 | 81.980 | 83.855 | 8.755  | 1.00 | 56.19 | E |
| ATOM | 5865 | CG  | ARG | E | 189 | 82.820 | 84.460 | 9.880  | 1.00 | 59.58 | E |
| ATOM | 5866 | CD  | ARG | E | 189 | 83.030 | 83.499 | 11.045 | 1.00 | 63.51 | E |
| ATOM | 5867 | NE  | ARG | E | 189 | 83.580 | 84.180 | 12.218 | 1.00 | 66.73 | E |
| ATOM | 5868 | CZ  | ARG | E | 189 | 84.771 | 84.771 | 12.255 | 1.00 | 68.44 | E |
| ATOM | 5869 | NH1 | ARG | E | 189 | 85.553 | 84.766 | 11.183 | 1.00 | 69.41 | E |
| ATOM | 5870 | NH2 | ARG | E | 189 | 85.178 | 85.378 | 13.363 | 1.00 | 70.13 | E |
| ATOM | 5871 | C   | ARG | E | 189 | 83.950 | 83.322 | 7.313  | 1.00 | 55.74 | E |
| ATOM | 5872 | O   | ARG | E | 189 | 85.043 | 83.182 | 7.866  | 1.00 | 56.16 | E |
| ATOM | 5873 | N   | ALA | E | 190 | 83.796 | 83.962 | 6.156  | 1.00 | 58.53 | E |
| ATOM | 5874 | CA  | ALA | E | 190 | 84.920 | 84.557 | 5.435  | 1.00 | 60.08 | E |
| ATOM | 5875 | CB  | ALA | E | 190 | 84.550 | 84.734 | 3.964  | 1.00 | 59.97 | E |
| ATOM | 5876 | C   | ALA | E | 190 | 85.335 | 85.905 | 6.036  | 1.00 | 61.01 | E |
| ATOM | 5877 | O   | ALA | E | 190 | 84.654 | 86.378 | 6.971  | 1.00 | 62.25 | E |
| ATOM | 5878 | OXT | ALA | E | 190 | 86.338 | 86.479 | 5.558  | 1.00 | 61.85 | E |
| ATOM | 5879 | C   | LEU | F | 1   | 78.718 | 38.094 | 33.366 | 1.00 | 32.03 | F |
| ATOM | 5880 | O   | LEU | F | 1   | 79.818 | 38.571 | 33.658 | 1.00 | 30.77 | F |
| ATOM | 5881 | N   | LEU | F | 1   | 76.219 | 38.100 | 33.307 | 1.00 | 33.21 | F |
| ATOM | 5882 | CA  | LEU | F | 1   | 77.432 | 38.678 | 33.953 | 1.00 | 32.59 | F |
| ATOM | 5883 | N   | GLN | F | 2   | 78.578 | 37.069 | 32.531 | 1.00 | 30.39 | F |
| ATOM | 5884 | CA  | GLN | F | 2   | 79.744 | 36.436 | 31.936 | 1.00 | 28.84 | F |
| ATOM | 5885 | C   | GLN | F | 2   | 79.609 | 36.081 | 30.462 | 1.00 | 27.93 | F |
| ATOM | 5886 | O   | GLN | F | 2   | 78.741 | 35.308 | 30.067 | 1.00 | 27.68 | F |
| ATOM | 5887 | N   | PRO | F | 3   | 80.463 | 36.663 | 29.619 | 1.00 | 28.02 | F |
| ATOM | 5888 | CD  | PRO | F | 3   | 81.461 | 37.720 | 29.856 | 1.00 | 28.68 | F |
| ATOM | 5889 | CA  | PRO | F | 3   | 80.370 | 36.332 | 28.198 | 1.00 | 27.76 | F |
| ATOM | 5890 | CB  | PRO | F | 3   | 81.363 | 37.298 | 27.552 | 1.00 | 28.01 | F |
| ATOM | 5891 | CG  | PRO | F | 3   | 82.353 | 37.575 | 28.660 | 1.00 | 28.41 | F |
| ATOM | 5892 | C   | PRO | F | 3   | 80.774 | 34.872 | 28.030 | 1.00 | 27.24 | F |
| ATOM | 5893 | O   | PRO | F | 3   | 81.698 | 34.406 | 28.698 | 1.00 | 27.18 | F |
| ATOM | 5894 | N   | PHE | F | 4   | 80.082 | 34.144 | 27.159 | 1.00 | 25.22 | F |
| ATOM | 5895 | CA  | PHE | F | 4   | 80.409 | 32.738 | 26.943 | 1.00 | 24.75 | F |
| ATOM | 5896 | CB  | PHE | F | 4   | 79.135 | 31.905 | 26.849 | 1.00 | 25.85 | F |
| ATOM | 5897 | CG  | PHE | F | 4   | 79.272 | 30.539 | 27.446 | 1.00 | 31.58 | F |
| ATOM | 5898 | CD1 | PHE | F | 4   | 79.435 | 30.384 | 28.823 | 1.00 | 33.24 | F |
| ATOM | 5899 | CD2 | PHE | F | 4   | 79.241 | 29.404 | 26.639 | 1.00 | 32.15 | F |
| ATOM | 5900 | CE1 | PHE | F | 4   | 79.561 | 29.116 | 29.386 | 1.00 | 33.28 | F |
| ATOM | 5901 | CE2 | PHE | F | 4   | 79.364 | 28.136 | 27.187 | 1.00 | 33.29 | F |
| ATOM | 5902 | CZ  | PHE | F | 4   | 79.524 | 27.989 | 28.565 | 1.00 | 34.18 | F |
| ATOM | 5903 | C   | PHE | F | 4   | 81.227 | 32.588 | 25.664 | 1.00 | 22.43 | F |
| ATOM | 5904 | O   | PHE | F | 4   | 80.759 | 32.919 | 24.586 | 1.00 | 24.59 | F |
| ATOM | 5905 | N   | PRO | F | 5   | 82.460 | 32.065 | 25.771 | 1.00 | 22.79 | F |
| ATOM | 5906 | CD  | PRO | F | 5   | 83.191 | 31.820 | 27.029 | 1.00 | 21.18 | F |
| ATOM | 5907 | CA  | PRO | F | 5   | 83.349 | 31.882 | 24.618 | 1.00 | 21.18 | F |
| ATOM | 5908 | CB  | PRO | F | 5   | 84.715 | 32.140 | 25.218 | 1.00 | 20.19 | F |
| ATOM | 5909 | CG  | PRO | F | 5   | 84.587 | 31.450 | 26.544 | 1.00 | 20.99 | F |
| ATOM | 5910 | C   | PRO | F | 5   | 83.291 | 30.524 | 23.949 | 1.00 | 20.28 | F |
| ATOM | 5911 | O   | PRO | F | 5   | 82.796 | 29.559 | 24.521 | 1.00 | 19.48 | F |
| ATOM | 5912 | N   | GLN | F | 6   | 83.818 | 30.456 | 22.730 | 1.00 | 21.24 | F |
| ATOM | 5913 | CA  | GLN | F | 6   | 83.848 | 29.200 | 21.983 | 1.00 | 19.98 | F |
| ATOM | 5914 | CB  | GLN | F | 6   | 83.665 | 29.450 | 20.484 | 1.00 | 18.71 | F |
| ATOM | 5915 | CG  | GLN | F | 6   | 82.312 | 30.010 | 20.048 | 1.00 | 18.35 | F |

| ATOM | 5916 | CD  | GLN | F | 6  | 82.255 | 30.247 | 18.537 | 1.00 | 22.29 | F |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 5917 | OE1 | GLN | F | 6  | 82.612 | 29.368 | 17.740 | 1.00 | 21.53 | F |
| ATOM | 5918 | NE2 | GLN | F | 6  | 81.802 | 31.429 | 18.138 | 1.00 | 20.02 | F |
| ATOM | 5919 | C   | GLN | F | 6  | 85.213 | 28.548 | 22.213 | 1.00 | 20.47 | F |
| ATOM | 5920 | O   | GLN | F | 6  | 86.243 | 29.204 | 22.099 | 1.00 | 18.48 | F |
| ATOM | 5921 | N   | PRO | F | 7  | 85.229 | 27.256 | 22.575 | 1.00 | 21.16 | F |
| ATOM | 5922 | CD  | PRO | F | 7  | 84.071 | 26.494 | 23.084 | 1.00 | 20.59 | F |
| ATOM | 5923 | CA  | PRO | F | 7  | 86.471 | 26.520 | 22.813 | 1.00 | 21.61 | F |
| ATOM | 5924 | CB  | PRO | F | 7  | 86.037 | 25.444 | 23.797 | 1.00 | 23.40 | F |
| ATOM | 5925 | CG  | PRO | F | 7  | 84.649 | 25.123 | 23.311 | 1.00 | 19.67 | F |
| ATOM | 5926 | C   | PRO | F | 7  | 86.996 | 25.897 | 21.521 | 1.00 | 23.00 | F |
| ATOM | 5927 | O   | PRO | F | 7  | 86.219 | 25.601 | 20.610 | 1.00 | 23.19 | F |
| ATOM | 5928 | N   | GLU | F | 8  | 88.312 | 25.714 | 21.438 | 1.00 | 21.78 | F |
| ATOM | 5929 | CA  | GLU | F | 8  | 88.904 | 25.068 | 20.279 | 1.00 | 23.12 | F |
| ATOM | 5930 | CB  | GLU | F | 8  | 90.297 | 25.632 | 19.968 | 1.00 | 24.50 | F |
| ATOM | 5931 | CG  | GLU | F | 8  | 91.086 | 24.834 | 18.915 | 1.00 | 26.16 | F |
| ATOM | 5932 | CD  | GLU | F | 8  | 90.360 | 24.697 | 17.576 | 1.00 | 31.57 | F |
| ATOM | 5933 | OE1 | GLU | F | 8  | 89.250 | 24.114 | 17.540 | 1.00 | 33.65 | F |
| ATOM | 5934 | OE2 | GLU | F | 8  | 90.903 | 25.171 | 16.555 | 1.00 | 30.66 | F |
| ATOM | 5935 | C   | GLU | F | 8  | 89.005 | 23.608 | 20.680 | 1.00 | 22.95 | F |
| ATOM | 5936 | O   | GLU | F | 8  | 89.289 | 23.292 | 21.833 | 1.00 | 23.25 | F |
| ATOM | 5937 | N   | LEU | F | 9  | 88.756 | 22.712 | 19.741 | 1.00 | 24.74 | F |
| ATOM | 5938 | CA  | LEU | F | 9  | 88.815 | 21.292 | 20.047 | 1.00 | 27.30 | F |
| ATOM | 5939 | CB  | LEU | F | 9  | 87.729 | 20.549 | 19.272 | 1.00 | 25.73 | F |
| ATOM | 5940 | CG  | LEU | F | 9  | 86.302 | 21.051 | 19.494 | 1.00 | 29.20 | F |
| ATOM | 5941 | CD1 | LEU | F | 9  | 85.338 | 20.235 | 18.645 | 1.00 | 28.18 | F |
| ATOM | 5942 | CD2 | LEU | F | 9  | 85.938 | 20.943 | 20.967 | 1.00 | 29.61 | F |
| ATOM | 5943 | C   | LEU | F | 9  | 90.178 | 20.707 | 19.712 | 1.00 | 28.17 | F |
| ATOM | 5944 | O   | LEU | F | 9  | 90.715 | 20.940 | 18.631 | 1.00 | 26.94 | F |
| ATOM | 5945 | N   | PRO | F | 10 | 90.765 | 19.947 | 20.647 | 1.00 | 30.38 | F |
| ATOM | 5946 | CD  | PRO | F | 10 | 90.365 | 19.707 | 22.044 | 1.00 | 30.47 | F |
| ATOM | 5947 | CA  | PRO | F | 10 | 92.076 | 19.355 | 20.370 | 1.00 | 34.24 | F |
| ATOM | 5948 | CB  | PRO | F | 10 | 92.556 | 18.915 | 21.752 | 1.00 | 32.97 | F |
| ATOM | 5949 | CG  | PRO | F | 10 | 91.282 | 18.561 | 22.448 | 1.00 | 31.98 | F |
| ATOM | 5950 | C   | PRO | F | 10 | 91.985 | 18.188 | 19.393 | 1.00 | 35.94 | F |
| ATOM | 5951 | O   | PRO | F | 10 | 90.993 | 17.461 | 19.376 | 1.00 | 38.70 | F |
| ATOM | 5952 | N   | TYR | F | 11 | 93.016 | 18.031 | 18.570 | 1.00 | 37.40 | F |
| ATOM | 5953 | CA  | TYR | F | 11 | 93.075 | 16.936 | 17.609 | 1.00 | 38.84 | F |
| ATOM | 5954 | CB  | TYR | F | 11 | 92.126 | 17.176 | 16.434 | 1.00 | 38.73 | F |
| ATOM | 5955 | CG  | TYR | F | 11 | 92.017 | 15.969 | 15.539 | 1.00 | 39.56 | F |
| ATOM | 5956 | CD1 | TYR | F | 11 | 91.294 | 14.848 | 15.942 | 1.00 | 39.88 | F |
| ATOM | 5957 | CE1 | TYR | F | 11 | 91.254 | 13.697 | 15.164 | 1.00 | 39.49 | F |
| ATOM | 5958 | CD2 | TYR | F | 11 | 92.698 | 15.913 | 14.327 | 1.00 | 39.73 | F |
| ATOM | 5959 | CE2 | TYR | F | 11 | 92.668 | 14.765 | 13.537 | 1.00 | 40.44 | F |
| ATOM | 5960 | CZ  | TYR | F | 11 | 91.945 | 13.659 | 13.964 | 1.00 | 40.29 | F |
| ATOM | 5961 | OH  | TYR | F | 11 | 91.921 | 12.514 | 13.200 | 1.00 | 40.03 | F |
| ATOM | 5962 | C   | TYR | F | 11 | 94.498 | 16.781 | 17.077 | 1.00 | 40.23 | F |
| ATOM | 5963 | O   | TYR | F | 11 | 95.102 | 15.708 | 17.300 | 1.00 | 41.88 | F |
| ATOM | 5964 | OXT | TYR | F | 11 | 94.988 | 17.742 | 16.443 | 1.00 | 40.58 | F |
| ATOM | 5965 | O   | HOH | H | 1  | 37.560 | 11.197 | 17.272 | 1.00 | 17.47 | H |
| ATOM | 5966 | O   | HOH | H | 2  | 81.295 | 26.543 | 20.573 | 1.00 | 15.95 | H |
| ATOM | 5967 | O   | HOH | H | 3  | 43.884 | 23.627 | 16.726 | 1.00 | 14.83 | H |
| ATOM | 5968 | O   | HOH | H | 4  | 89.230 | 61.015 | 16.512 | 1.00 | 19.10 | H |
| ATOM | 5969 | O   | HOH | H | 5  | 92.090 | 40.877 | 18.768 | 1.00 | 15.59 | H |
| ATOM | 5970 | O   | HOH | H | 6  | 57.686 | 14.054 | 4.407  | 1.00 | 20.02 | H |
| ATOM | 5971 | O   | HOH | H | 7  | 87.607 | 31.423 | 22.217 | 1.00 | 11.29 | H |
| ATOM | 5972 | O   | HOH | H | 8  | 31.815 | 41.479 | 5.673  | 1.00 | 23.91 | H |
| ATOM | 5973 | O   | HOH | H | 9  | 46.112 | 3.594  | 18.714 | 1.00 | 20.15 | H |
| ATOM | 5974 | O   | HOH | H | 10 | 86.724 | 67.786 | 15.551 | 1.00 | 22.39 | H |
| ATOM | 5975 | O   | HOH | H | 11 | 42.599 | 14.833 | 17.213 | 1.00 | 16.12 | H |
| ATOM | 5976 | O   | HOH | H | 12 | 93.679 | 37.081 | 11.737 | 1.00 | 15.03 | H |
| ATOM | 5977 | O   | HOH | H | 13 | 50.288 | 0.581  | 25.262 | 1.00 | 13.69 | H |
| ATOM | 5978 | O   | HOH | H | 14 | 96.256 | 37.853 | 25.291 | 1.00 | 12.90 | H |
| ATOM | 5979 | O   | HOH | H | 15 | 90.711 | 30.936 | 37.307 | 1.00 | 31.88 | H |
| ATOM | 5980 | O   | HOH | H | 16 | 80.045 | 39.846 | 25.144 | 1.00 | 33.11 | H |
| ATOM | 5981 | O   | HOH | H | 17 | 80.708 | 45.662 | 11.514 | 1.00 | 41.56 | H |
| ATOM | 5982 | O   | HOH | H | 18 | 42.215 | 0.119  | 11.193 | 1.00 | 15.83 | H |
| ATOM | 5983 | O   | HOH | H | 19 | 95.828 | 50.485 | 5.930  | 1.00 | 27.67 | H |
| ATOM | 5984 | O   | HOH | H | 20 | 48.809 | 37.278 | 14.928 | 1.00 | 36.10 | H |
| ATOM | 5985 | O   | HOH | H | 21 | 47.553 | -0.403 | 11.823 | 1.00 | 14.62 | H |
| ATOM | 5986 | O   | HOH | H | 22 | 94.554 | 76.132 | 19.122 | 1.00 | 83.80 | H |
| ATOM | 5987 | O   | HOH | H | 23 | 83.295 | 48.460 | 17.328 | 1.00 | 17.64 | H |
| ATOM | 5988 | O   | HOH | H | 24 | 88.976 | 42.102 | 7.818  | 1.00 | 26.11 | H |
| ATOM | 5989 | O   | HOH | H | 25 | 99.041 | 56.322 | 24.823 | 1.00 | 24.86 | H |

| ATOM | 5990 | O | HOH H | 26 | 47.640 | 0.006 | 20.312 | 1.00 18.95 | H |
|------|------|---|-------|----|--------|-------|--------|------------|---|
| ATOM | 5991 | O | HOH H | 27 | 46.987 | 29.359 | 11.916 | 1.00 21.84 | H |
| ATOM | 5992 | O | HOH H | 28 | 88.283 | 37.229 | 11.279 | 1.00 21.34 | H |
| ATOM | 5993 | O | HOH H | 29 | 49.878 | -9.043 | 36.424 | 1.00 32.47 | H |
| ATOM | 5994 | O | HOH H | 30 | 82.777 | 39.366 | 24.935 | 1.00 24.79 | H |
| ATOM | 5995 | O | HOH H | 31 | 72.919 | 25.704 | 15.123 | 1.00 18.09 | H |
| ATOM | 5996 | O | HOH H | 32 | 86.830 | 25.153 | 13.558 | 1.00 24.14 | H |
| ATOM | 5997 | O | HOH H | 33 | 43.152 | 5.651 | 13.774 | 1.00 19.96 | H |
| ATOM | 5998 | O | HOH H | 34 | 100.654 | 27.732 | 5.367 | 1.00 34.73 | H |
| ATOM | 5999 | O | HOH H | 35 | 48.550 | 32.122 | 26.894 | 1.00 20.17 | H |
| ATOM | 6000 | O | HOH H | 36 | 78.728 | 36.578 | 6.822 | 1.00 32.92 | H |
| ATOM | 6001 | O | HOH H | 37 | 89.361 | 11.980 | 24.953 | 1.00 51.75 | H |
| ATOM | 6002 | O | HOH H | 38 | 90.411 | 24.657 | 31.926 | 1.00 28.29 | H |
| ATOM | 6003 | O | HOH H | 39 | 80.690 | 24.233 | 8.462 | 1.00 22.43 | H |
| ATOM | 6004 | O | HOH H | 40 | 83.769 | 65.973 | -5.489 | 1.00 21.06 | H |
| ATOM | 6005 | O | HOH H | 41 | 87.710 | 34.692 | 7.008 | 1.00 22.47 | H |
| ATOM | 6006 | O | HOH H | 42 | 38.997 | 4.521 | 15.299 | 1.00 25.36 | H |
| ATOM | 6007 | O | HOH H | 43 | 94.223 | 46.644 | 24.674 | 1.00 32.67 | H |
| ATOM | 6008 | O | HOH H | 44 | 35.150 | 15.757 | 26.294 | 1.00 29.03 | H |
| ATOM | 6009 | O | HOH H | 45 | 85.059 | 24.652 | 18.280 | 1.00 25.63 | H |
| ATOM | 6010 | O | HOH H | 46 | 67.739 | 6.320 | 18.991 | 1.00 43.67 | H |
| ATOM | 6011 | O | HOH H | 47 | 92.376 | 63.977 | 12.866 | 1.00 32.46 | H |
| ATOM | 6012 | O | HOH H | 48 | 91.526 | 49.479 | 22.504 | 1.00 29.70 | H |
| ATOM | 6013 | O | HOH H | 49 | 56.333 | -2.088 | 24.733 | 1.00 28.53 | H |
| ATOM | 6014 | O | HOH H | 50 | 100.482 | 53.937 | 3.942 | 1.00 52.26 | H |
| ATOM | 6015 | O | HOH H | 51 | 48.244 | 18.753 | 22.918 | 1.00 44.88 | H |
| ATOM | 6016 | O | HOH H | 52 | 32.577 | -0.558 | 6.769 | 1.00 33.70 | H |
| ATOM | 6017 | O | HOH H | 53 | 47.162 | 26.527 | 12.972 | 1.00 29.72 | H |
| ATOM | 6018 | O | HOH H | 54 | 98.621 | 66.834 | 5.100 | 1.00 52.20 | H |
| ATOM | 6019 | O | HOH H | 55 | 88.106 | 52.134 | 17.293 | 1.00 21.13 | H |
| ATOM | 6020 | O | HOH H | 56 | 59.655 | 31.307 | 17.069 | 1.00 25.89 | H |
| ATOM | 6021 | O | HOH H | 57 | 73.562 | 24.323 | 12.997 | 1.00 23.51 | H |
| ATOM | 6022 | O | HOH H | 58 | 43.748 | 32.725 | 20.165 | 1.00 52.72 | H |
| ATOM | 6023 | O | HOH H | 59 | 26.392 | -7.072 | 11.400 | 1.00 26.20 | H |
| ATOM | 6024 | O | HOH H | 60 | 83.955 | 73.751 | 16.805 | 1.00 18.19 | H |
| ATOM | 6025 | O | HOH H | 61 | 46.229 | -19.766 | 10.675 | 1.00 28.79 | H |
| ATOM | 6026 | O | HOH H | 62 | 52.436 | 38.720 | 16.630 | 1.00 28.35 | H |
| ATOM | 6027 | O | HOH H | 63 | 60.555 | 9.392 | 19.914 | 1.00 28.43 | H |
| ATOM | 6028 | O | HOH H | 64 | 62.105 | 2.197 | 11.948 | 1.00 33.33 | H |
| ATOM | 6029 | O | HOH H | 65 | 40.514 | -12.059 | 13.631 | 1.00 21.32 | H |
| ATOM | 6030 | O | HOH H | 66 | 65.876 | 23.972 | 14.155 | 1.00 21.11 | H |
| ATOM | 6031 | O | HOH H | 67 | 84.702 | 18.013 | 5.666 | 1.00 19.12 | H |
| ATOM | 6032 | O | HOH H | 68 | 64.715 | 11.655 | 15.936 | 1.00 28.72 | H |
| ATOM | 6033 | O | HOH H | 69 | 85.418 | 74.949 | 14.820 | 1.00 27.90 | H |
| ATOM | 6034 | O | HOH H | 70 | 77.974 | 25.419 | 23.038 | 1.00 42.15 | H |
| ATOM | 6035 | O | HOH H | 71 | 65.805 | 8.484 | 20.741 | 1.00 44.01 | H |
| ATOM | 6036 | O | HOH H | 72 | 51.276 | 26.045 | 10.800 | 1.00 28.36 | H |
| ATOM | 6037 | O | HOH H | 73 | 65.226 | 22.195 | 25.831 | 1.00 36.11 | H |
| ATOM | 6038 | O | HOH H | 74 | 101.567 | 46.068 | 1.107 | 1.00 53.81 | H |
| ATOM | 6039 | O | HOH H | 75 | 32.615 | 31.234 | 1.517 | 1.00 21.03 | H |
| ATOM | 6040 | O | HOH H | 76 | 42.100 | -0.001 | 13.802 | 1.00 23.44 | H |
| ATOM | 6041 | O | HOH H | 77 | 35.124 | 40.614 | 14.668 | 1.00 27.61 | H |
| ATOM | 6042 | O | HOH H | 78 | 92.548 | 46.813 | 7.595 | 1.00 31.64 | H |
| ATOM | 6043 | O | HOH H | 79 | 34.670 | 13.941 | 14.778 | 1.00 22.87 | H |
| ATOM | 6044 | O | HOH H | 80 | 98.527 | 27.671 | 28.270 | 1.00 42.07 | H |
| ATOM | 6045 | O | HOH H | 81 | 30.588 | 36.032 | 16.540 | 1.00 37.52 | H |
| ATOM | 6046 | O | HOH H | 82 | 89.345 | 42.957 | 13.940 | 1.00 22.73 | H |
| ATOM | 6047 | O | HOH H | 83 | 92.891 | 18.085 | 10.698 | 1.00 32.35 | H |
| ATOM | 6048 | O | HOH H | 84 | 90.050 | 48.556 | 16.519 | 1.00 27.30 | H |
| ATOM | 6049 | O | HOH H | 85 | 110.812 | 49.549 | 15.813 | 1.00 27.68 | H |
| ATOM | 6050 | O | HOH H | 86 | 75.872 | 21.668 | 2.499 | 1.00 39.37 | H |
| ATOM | 6051 | O | HOH H | 87 | 52.567 | 14.010 | 7.270 | 1.00 34.20 | H |
| ATOM | 6052 | O | HOH H | 88 | 69.016 | 32.569 | 12.651 | 1.00 36.96 | H |
| ATOM | 6053 | O | HOH H | 89 | 96.637 | 25.945 | 31.742 | 1.00 37.26 | H |
| ATOM | 6054 | O | HOH H | 90 | 34.496 | -12.998 | 8.560 | 1.00 22.82 | H |
| ATOM | 6055 | O | HOH H | 91 | 113.021 | 48.469 | 17.945 | 1.00 47.59 | H |
| ATOM | 6056 | O | HOH H | 92 | 34.266 | 25.052 | 23.930 | 1.00 31.02 | H |
| ATOM | 6057 | O | HOH H | 93 | 51.464 | 31.946 | 19.300 | 1.00 15.75 | H |
| ATOM | 6058 | O | HOH H | 94 | 80.054 | 50.912 | 15.041 | 1.00 25.94 | H |
| ATOM | 6059 | O | HOH H | 95 | 40.413 | -13.432 | 16.393 | 1.00 39.73 | H |
| ATOM | 6060 | O | HOH H | 96 | 57.701 | 4.191 | 7.708 | 1.00 25.27 | H |
| ATOM | 6061 | O | HOH H | 97 | 80.838 | 52.853 | 26.436 | 1.00 27.67 | H |
| ATOM | 6062 | O | HOH H | 98 | 58.205 | 13.023 | 20.294 | 1.00 27.57 | H |
| ATOM | 6063 | O | HOH H | 99 | 41.832 | 30.497 | 15.601 | 1.00 27.32 | H |

| ATOM | 6064 | O | HOH H 100 | 72.807 | 29.880 | 11.618 | 1.00 | 28.05 | H |
|------|------|---|-----------|--------|--------|--------|------|-------|---|
| ATOM | 6065 | O | HOH H 101 | 48.499 | 5.079 | 4.053 | 1.00 | 38.72 | H |
| ATOM | 6066 | O | HOH H 102 | 100.679 | 66.408 | 9.019 | 1.00 | 36.21 | H |
| ATOM | 6067 | O | HOH H 103 | 45.023 | 41.442 | 11.747 | 1.00 | 42.72 | H |
| ATOM | 6068 | O | HOH H 104 | 83.296 | 63.483 | -2.738 | 1.00 | 27.46 | H |
| ATOM | 6069 | O | HOH H 105 | 85.067 | 29.522 | 34.732 | 1.00 | 35.62 | H |
| ATOM | 6070 | O | HOH H 106 | 72.272 | 53.390 | 15.314 | 1.00 | 38.75 | H |
| ATOM | 6071 | O | HOH H 107 | 80.600 | 27.688 | 5.225 | 1.00 | 26.04 | H |
| ATOM | 6072 | O | HOH H 108 | 71.251 | 18.567 | 16.503 | 1.00 | 29.08 | H |
| ATOM | 6073 | O | HOH H 109 | 88.274 | 65.356 | 19.510 | 1.00 | 26.70 | H |
| ATOM | 6074 | O | HOH H 110 | 43.031 | 4.836 | 7.813 | 1.00 | 38.59 | H |
| ATOM | 6075 | O | HOH H 111 | 101.304 | 35.384 | 4.755 | 1.00 | 43.53 | H |
| ATOM | 6076 | O | HOH H 112 | 44.554 | 10.725 | 19.619 | 1.00 | 21.38 | H |
| ATOM | 6077 | O | HOH H 113 | 115.506 | 34.478 | 5.615 | 1.00 | 46.62 | H |
| ATOM | 6078 | O | HOH H 114 | 36.124 | -25.634 | 9.802 | 1.00 | 42.69 | H |
| ATOM | 6079 | O | HOH H 115 | 34.494 | -33.304 | 20.170 | 1.00 | 61.12 | H |
| ATOM | 6080 | O | HOH H 116 | 38.663 | 26.161 | -2.715 | 1.00 | 31.39 | H |
| ATOM | 6081 | O | HOH H 117 | 105.197 | 41.384 | 18.739 | 1.00 | 38.53 | H |
| ATOM | 6082 | O | HOH H 118 | 38.437 | -12.372 | 18.422 | 1.00 | 32.47 | H |
| ATOM | 6083 | O | HOH H 119 | 45.430 | 15.732 | 9.556 | 1.00 | 32.39 | H |
| ATOM | 6084 | O | HOH H 120 | 70.475 | 9.817 | -1.029 | 1.00 | 53.38 | H |
| ATOM | 6085 | O | HOH H 121 | 87.895 | 64.540 | 22.445 | 1.00 | 47.01 | H |
| ATOM | 6086 | O | HOH H 122 | 39.337 | 36.650 | 16.644 | 1.00 | 25.21 | H |
| ATOM | 6087 | O | HOH H 123 | 104.091 | 50.783 | 20.204 | 1.00 | 31.31 | H |
| ATOM | 6088 | O | HOH H 124 | 72.528 | 13.825 | 20.909 | 1.00 | 62.81 | H |
| ATOM | 6089 | O | HOH H 125 | 55.353 | -5.411 | 5.747 | 1.00 | 25.46 | H |
| ATOM | 6090 | O | HOH H 126 | 97.848 | 63.704 | 25.177 | 1.00 | 27.84 | H |
| ATOM | 6091 | O | HOH H 127 | 89.799 | 75.117 | 14.074 | 1.00 | 49.56 | H |
| ATOM | 6092 | O | HOH H 128 | 96.226 | 35.565 | 0.211 | 1.00 | 40.25 | H |
| ATOM | 6093 | O | HOH H 129 | 25.125 | -15.445 | 19.161 | 1.00 | 37.04 | H |
| ATOM | 6094 | O | HOH H 130 | 90.627 | 52.974 | 9.649 | 1.00 | 22.70 | H |
| ATOM | 6095 | O | HOH H 131 | 114.398 | 29.773 | 11.425 | 1.00 | 42.36 | H |
| ATOM | 6096 | O | HOH H 132 | 69.810 | 89.608 | -0.164 | 1.00 | 53.48 | H |
| ATOM | 6097 | O | HOH H 133 | 99.069 | 30.421 | 4.728 | 1.00 | 31.21 | H |
| ATOM | 6098 | O | HOH H 134 | 37.335 | 49.129 | 5.746 | 1.00 | 43.90 | H |
| ATOM | 6099 | O | HOH H 135 | 77.753 | 73.821 | 17.600 | 1.00 | 50.43 | H |
| ATOM | 6100 | O | HOH H 136 | 44.853 | 33.208 | 11.090 | 1.00 | 21.26 | H |
| ATOM | 6101 | O | HOH H 137 | 88.697 | 80.608 | -4.574 | 1.00 | 49.42 | H |
| ATOM | 6102 | O | HOH H 138 | 62.018 | -6.136 | 9.010 | 1.00 | 30.19 | H |
| ATOM | 6103 | O | HOH H 139 | 35.964 | -5.810 | 5.494 | 1.00 | 45.47 | H |
| ATOM | 6104 | O | HOH H 140 | 73.968 | 65.480 | 8.013 | 1.00 | 43.93 | H |
| ATOM | 6105 | O | HOH H 141 | 78.361 | 66.868 | 24.455 | 1.00 | 57.76 | H |
| ATOM | 6106 | O | HOH H 142 | 53.527 | 3.199 | 22.332 | 1.00 | 32.95 | H |
| ATOM | 6107 | O | HOH H 143 | 56.018 | -6.530 | 25.205 | 1.00 | 42.75 | H |
| ATOM | 6108 | O | HOH H 144 | 82.930 | 52.617 | 28.345 | 1.00 | 32.35 | H |
| ATOM | 6109 | O | HOH H 145 | 28.607 | -21.313 | 24.210 | 1.00 | 48.87 | H |
| ATOM | 6110 | O | HOH H 146 | 86.079 | 41.197 | 35.698 | 1.00 | 36.97 | H |
| ATOM | 6111 | O | HOH H 147 | 35.017 | 8.399 | 11.516 | 1.00 | 32.21 | H |
| ATOM | 6112 | O | HOH H 148 | 25.864 | -19.905 | 17.166 | 1.00 | 41.53 | H |
| ATOM | 6113 | O | HOH H 149 | 55.504 | 20.659 | 6.959 | 1.00 | 36.63 | H |
| ATOM | 6114 | O | HOH H 150 | 106.046 | 47.260 | 19.571 | 1.00 | 30.60 | H |
| ATOM | 6115 | O | HOH H 151 | 108.769 | 26.147 | 5.447 | 1.00 | 48.82 | H |
| ATOM | 6116 | O | HOH H 152 | 38.689 | 17.576 | 4.331 | 1.00 | 39.07 | H |
| ATOM | 6117 | O | HOH H 153 | 97.787 | 62.580 | 8.740 | 1.00 | 29.61 | H |
| ATOM | 6118 | O | HOH H 154 | 59.501 | -12.817 | 20.769 | 1.00 | 50.36 | H |
| ATOM | 6119 | O | HOH H 155 | 47.887 | 40.072 | -4.641 | 1.00 | 51.05 | H |
| ATOM | 6120 | O | HOH H 156 | 60.057 | 16.564 | 27.477 | 1.00 | 40.66 | H |
| ATOM | 6121 | O | HOH H 157 | 67.048 | 27.841 | 20.873 | 1.00 | 39.66 | H |
| ATOM | 6122 | O | HOH H 158 | 37.028 | 32.932 | 18.669 | 1.00 | 37.23 | H |
| ATOM | 6123 | O | HOH H 159 | 121.780 | 18.693 | -3.076 | 1.00 | 46.64 | H |
| ATOM | 6124 | O | HOH H 160 | 39.196 | 18.091 | 27.271 | 1.00 | 29.99 | H |
| ATOM | 6125 | O | HOH H 161 | 113.285 | 44.237 | 19.561 | 1.00 | 39.04 | H |
| ATOM | 6126 | O | HOH H 162 | 43.379 | 27.754 | 19.370 | 1.00 | 27.58 | H |
| ATOM | 6127 | O | HOH H 163 | 91.636 | 66.903 | 11.885 | 1.00 | 54.73 | H |
| ATOM | 6128 | O | HOH H 164 | 113.381 | 46.844 | 20.020 | 1.00 | 54.22 | H |
| ATOM | 6129 | O | HOH H 165 | 79.238 | 62.082 | 24.112 | 1.00 | 36.07 | H |
| ATOM | 6130 | O | HOH H 166 | 27.985 | 32.355 | 18.424 | 1.00 | 36.25 | H |
| ATOM | 6131 | O | HOH H 167 | 34.709 | -10.661 | 20.615 | 1.00 | 9.89 | H |
| ATOM | 6132 | O | HOH H 168 | 93.577 | 37.339 | 20.182 | 1.00 | 14.03 | H |
| ATOM | 6133 | O | HOH H 169 | 97.912 | 51.662 | 7.309 | 1.00 | 24.22 | H |
| ATOM | 6134 | O | HOH H 170 | 69.616 | 4.375 | 18.521 | 1.00 | 38.01 | H |
| ATOM | 6135 | O | HOH H 171 | 80.870 | 25.194 | 6.002 | 1.00 | 21.84 | H |
| ATOM | 6136 | O | HOH H 172 | 50.564 | 12.887 | 5.906 | 1.00 | 32.25 | H |
| ATOM | 6137 | O | HOH H 173 | 88.207 | 37.288 | 13.919 | 1.00 | 19.68 | H |

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ATOM    6138   O   HOH H 174    93.800  47.651  27.174  1.00 41.65       H
ATOM    6139   O   HOH H 175    52.842   0.304  25.210  1.00 28.07       H
ATOM    6140   O   HOH H 176    66.457   4.742  14.051  1.00 28.64       H
ATOM    6141   O   HOH H 177    36.948  12.416  15.109  1.00 28.66       H
ATOM    6142   O   HOH H 178   103.292  41.793   7.607  1.00 28.51       H
ATOM    6143   O   HOH H 179    86.476  36.035   9.339  1.00 27.43       H
ATOM    6144   O   HOH H 180    82.262  41.159  26.845  1.00 24.13       H
ATOM    6145   O   HOH H 181    32.348  15.030  26.400  1.00 30.06       H
ATOM    6146   O   HOH H 182    69.916  30.709  14.482  1.00 42.81       H
ATOM    6147   O   HOH H 183    48.060  10.142  26.751  1.00 49.12       H
ATOM    6148   O   HOH H 184    45.863  -9.131  37.252  1.00 43.70       H
ATOM    6149   O   HOH H 185    32.095  -3.806  34.251  1.00 41.46       H
ATOM    6150   O   HOH H 186   108.258  31.975   8.914  1.00 33.62       H
ATOM    6151   O   HOH H 187    99.465  64.293   8.210  1.00 54.43       H
ATOM    6152   O   HOH H 188    74.677  30.785  27.841  1.00 28.20       H
ATOM    6153   O   HOH H 189    44.953   0.968  35.892  1.00 32.25       H
ATOM    6154   O   HOH H 190    88.523  27.792  36.268  1.00 30.83       H
ATOM    6155   O   HOH H 191    37.736   8.611  11.729  1.00 38.92       H
ATOM    6156   O   HOH H 192    35.988  45.178  12.964  1.00 33.85       H
ATOM    6157   O   HOH H 193    77.222  68.027   1.401  1.00 27.02       H
ATOM    6158   O   HOH H 194    63.326  -8.764  15.926  1.00 38.46       H
ATOM    6159   O   HOH H 195   109.635  61.489  27.644  1.00 52.79       H
ATOM    6160   O   HOH H 196   101.299  67.528  11.319  1.00 38.92       H
ATOM    6161   O   HOH H 197    77.295  56.116  25.768  1.00 36.83       H
ATOM    6162   O   HOH H 198    81.538  22.288   0.320  1.00 47.08       H
ATOM    6163   O   HOH H 199    55.989   3.900   0.756  1.00 46.35       H
ATOM    6164   O   HOH H 200    66.200  40.514  17.513  1.00 43.54       H
ATOM    6165   O   HOH H 201    40.497  -1.046   9.238  1.00 27.84       H
ATOM    6166   O   HOH H 202    57.171  27.504   8.258  1.00 52.74       H
ATOM    6167   O   HOH H 203    44.592  -6.430  37.531  1.00 37.55       H
ATOM    6168   O   HOH H 204    26.892  -1.642   9.494  1.00 55.58       H
ATOM    6169   O   HOH H 205    83.350  58.389   2.759  1.00 46.24       H
ATOM    6170   O   HOH H 206   112.353  45.284   9.770  1.00 30.99       H
ATOM    6171   O   HOH H 207    86.315  23.927  16.100  1.00 41.36       H
ATOM    6172   O   HOH H 208    67.053  45.396  12.396  1.00 31.02       H
ATOM    6173   O   HOH H 209   111.609  60.418   8.362  1.00 52.01       H
ATOM    6174   O   HOH H 210    91.254  47.553  32.752  1.00 41.71       H
ATOM    6175   O   HOH H 211    88.489  39.944  11.117  1.00 34.00       H
ATOM    6176   O   HOH H 212   104.972  69.233  16.415  1.00 37.26       H
ATOM    6177   O   HOH H 213    23.462  39.893   6.692  1.00 56.45       H
ATOM    6178   O   HOH H 214    84.114  54.447  -1.718  1.00 42.58       H
ATOM    6179   O   HOH H 215   105.045  66.068  22.775  1.00 24.48       H
ATOM    6180   O   HOH H 216    85.378  52.388  17.025  1.00 37.91       H
ATOM    6181   O   HOH H 217    91.411  30.837   4.259  1.00 23.59       H
ATOM    6182   O   HOH H 218    99.019  37.803  25.178  1.00 37.20       H
ATOM    6183   O   HOH H 219    88.866  41.183  35.781  1.00 42.88       H
ATOM    6184   O   HOH H 220    66.946  25.931  12.530  1.00 45.53       H
ATOM    6185   O   HOH H 221    83.809  61.544  -0.645  1.00 32.51       H
ATOM    6186   O   HOH H 222    91.766  28.386   3.286  1.00 29.97       H
ATOM    6187   O   HOH H 223    83.302  45.674  11.423  1.00 40.65       H
ATOM    6188   O   HOH H 224    59.198   3.628  18.904  1.00 22.61       H
ATOM    6189   O   HOH H 225    34.553 -11.852   5.930  1.00 29.77       H
ATOM    6190   O   HOH H 226    88.953  22.712  24.560  1.00 23.54       H
ATOM    6191   O   HOH H 227   108.379  54.102  21.160  1.00 30.79       H
ATOM    6192   O   HOH H 228    44.957  16.820   6.827  1.00 37.14       H
ATOM    6193   O   HOH H 229   105.872  50.217  22.393  1.00 33.77       H
ATOM    6194   O   HOH H 230    40.390  52.287  -1.729  1.00 62.00       H
ATOM    6195   O   HOH H 231   103.837  27.586  24.806  1.00 50.76       H
ATOM    6196   O   HOH H 232    50.931   9.397  25.207  1.00 40.65       H
ATOM    6197   O   HOH H 233    64.739   2.382  27.973  1.00 46.98       H
ATOM    6198   O   HOH H 234    38.363   0.460   8.402  1.00 28.58       H
ATOM    6199   O   HOH H 235    73.577  50.129  18.561  1.00 36.68       H
ATOM    6200   O   HOH H 236   100.912  58.519   6.876  1.00 36.99       H
ATOM    6201   O   HOH H 237   100.664  26.841  26.380  1.00 36.27       H
ATOM    6202   O   HOH H 238    82.528  48.080  12.484  1.00 44.97       H
ATOM    6203   O   HOH H 239    70.870  44.782  13.746  1.00 26.53       H
ATOM    6204   O   HOH H 240    71.914  -9.049  17.302  1.00 59.29       H
ATOM    6205   O   HOH H 241    28.024   9.146  32.377  1.00 43.91       H
ATOM    6206   O   HOH H 242    55.531  -2.470   4.880  1.00 50.20       H
ATOM    6207   O   HOH H 243    63.362  16.623  21.334  1.00 30.95       H
ATOM    6208   O   HOH H 244    71.813  27.548  12.914  1.00 54.77       H
ATOM    6209   O   HOH H 245    22.793  -3.930  12.731  1.00 39.10       H
ATOM    6210   O   HOH H 246    73.087  44.091  34.124  1.00 47.86       H
ATOM    6211   O   HOH H 247    48.717  31.774  19.850  1.00 33.46       H
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| ATOM | 6212 | O | HOH H 248 | 100.851 | 61.218 | 7.741 | 1.00 | 35.49 | H |
|------|------|---|-----------|---------|--------|-------|------|-------|---|
| ATOM | 6213 | O | HOH H 249 | 116.291 | 47.311 | 12.227 | 1.00 | 49.67 | H |
| ATOM | 6214 | O | HOH H 250 | 99.469 | 40.748 | 22.418 | 1.00 | 25.82 | H |
| ATOM | 6215 | O | HOH H 251 | 52.271 | 4.031 | 24.614 | 1.00 | 44.68 | H |
| ATOM | 6216 | O | HOH H 252 | 106.629 | 40.298 | 32.271 | 1.00 | 59.44 | H |
| ATOM | 6217 | O | HOH H 253 | 45.587 | -9.303 | 3.049 | 1.00 | 26.81 | H |
| ATOM | 6218 | O | HOH H 254 | 52.547 | -9.432 | 27.670 | 1.00 | 45.08 | H |
| ATOM | 6219 | O | HOH H 255 | 75.854 | 21.157 | 27.640 | 1.00 | 42.33 | H |
| ATOM | 6220 | O | HOH H 256 | 82.119 | 63.444 | 23.430 | 1.00 | 37.84 | H |
| ATOM | 6221 | O | HOH H 257 | 104.091 | 38.660 | 18.936 | 1.00 | 30.29 | H |
| ATOM | 6222 | O | HOH H 258 | 79.477 | 56.121 | 8.190 | 1.00 | 39.16 | H |
| ATOM | 6223 | O | HOH H 259 | 101.351 | 32.257 | 5.631 | 1.00 | 29.94 | H |
| ATOM | 6224 | O | HOH H 260 | 93.989 | 23.313 | 31.488 | 1.00 | 35.30 | H |
| ATOM | 6225 | O | HOH H 261 | 28.754 | -1.723 | 6.977 | 1.00 | 36.90 | H |
| ATOM | 6226 | O | HOH H 262 | 93.007 | 48.370 | 9.901 | 1.00 | 49.06 | H |
| ATOM | 6227 | O | HOH H 263 | 82.990 | 88.137 | 9.529 | 1.00 | 39.70 | H |
| ATOM | 6228 | O | HOH H 264 | 118.031 | 51.582 | 0.542 | 1.00 | 36.21 | H |
| ATOM | 6229 | O | HOH H 265 | 21.682 | 15.046 | 11.602 | 1.00 | 62.29 | H |
| ATOM | 6230 | O | HOH H 266 | 34.210 | 24.576 | 5.314 | 1.00 | 18.89 | H |
| ATOM | 6231 | O | HOH H 267 | 85.829 | 40.095 | 14.911 | 1.00 | 25.26 | H |
| ATOM | 6232 | O | HOH H 268 | 102.070 | 38.308 | 21.059 | 1.00 | 41.79 | H |
| ATOM | 6233 | O | HOH H 269 | 41.071 | -2.346 | 7.039 | 1.00 | 38.87 | H |
| ATOM | 6234 | O | HOH H 270 | 68.717 | 3.686 | 16.083 | 1.00 | 37.79 | H |
| ATOM | 6235 | O | HOH H 271 | 27.094 | -12.649 | 12.753 | 1.00 | 29.26 | H |
| ATOM | 6236 | O | HOH H 272 | 36.426 | 24.744 | 4.145 | 1.00 | 45.88 | H |
| ATOM | 6237 | O | HOH H 273 | 88.670 | 31.858 | 5.525 | 1.00 | 39.43 | H |
| ATOM | 6238 | O | HOH H 274 | 90.819 | 38.524 | 36.028 | 1.00 | 30.15 | H |
| ATOM | 6239 | O | HOH H 275 | 90.790 | 49.861 | 10.317 | 1.00 | 39.97 | H |
| ATOM | 6240 | O | HOH H 276 | 77.026 | 11.969 | 13.970 | 1.00 | 44.87 | H |
| ATOM | 6241 | O | HOH H 277 | 36.555 | 12.078 | 12.344 | 1.00 | 40.47 | H |
| ATOM | 6242 | O | HOH H 278 | 52.331 | 7.302 | 24.972 | 1.00 | 49.30 | H |
| ATOM | 6243 | O | HOH H 279 | 92.612 | 33.229 | 3.564 | 1.00 | 40.55 | H |
| ATOM | 6244 | O | HOH H 280 | 83.546 | 64.142 | 25.612 | 1.00 | 50.28 | H |
| ATOM | 6245 | O | HOH H 281 | 28.206 | -1.891 | 36.868 | 1.00 | 44.06 | H |
| ATOM | 6246 | O | HOH H 282 | 93.185 | 20.914 | 30.917 | 1.00 | 44.51 | H |
| ATOM | 6247 | O | HOH H 283 | 98.176 | 41.763 | 24.500 | 1.00 | 44.20 | H |
| ATOM | 6248 | O | HOH H 284 | 29.174 | -0.123 | 4.304 | 1.00 | 46.75 | H |
| ATOM | 6249 | O | HOH H 285 | 79.206 | 77.643 | 14.919 | 1.00 | 30.21 | H |
| ATOM | 6250 | O | HOH H 286 | 90.531 | 26.085 | 37.436 | 1.00 | 36.96 | H |
| ATOM | 6251 | O | HOH H 287 | 55.726 | 0.396 | 21.054 | 1.00 | 49.55 | H |
| ATOM | 6252 | O | HOH H 288 | 111.246 | 30.915 | 19.699 | 1.00 | 42.91 | H |
| ATOM | 6253 | O | HOH H 289 | 77.000 | 58.921 | 5.300 | 1.00 | 47.04 | H |
| ATOM | 6254 | O, | HOH H 290 | 34.339 | -9.458 | 5.288 | 1.00 | 25.50 | H |
| ATOM | 6255 | O | HOH H 291 | 109.784 | 29.168 | 15.534 | 1.00 | 45.96 | H |
| ATOM | 6256 | O | HOH H 292 | 93.674 | 48.853 | 29.650 | 1.00 | 48.76 | H |
| ATOM | 6257 | O | HOH H 293 | 92.299 | 47.066 | 3.801 | 1.00 | 37.41 | H |
| ATOM | 6258 | O | HOH H 294 | 110.965 | 23.141 | 11.799 | 1.00 | 42.97 | H |
| ATOM | 6259 | O | HOH H 295 | 90.562 | 45.235 | 33.919 | 1.00 | 33.83 | H |
| ATOM | 6260 | O | HOH H 296 | 57.772 | -10.500 | 25.018 | 1.00 | 49.78 | H |
| ATOM | 6261 | O | HOH H 297 | 54.676 | 36.195 | 11.362 | 1.00 | 54.22 | H |
| ATOM | 6262 | O | HOH H 298 | 107.263 | 59.234 | 5.282 | 1.00 | 56.05 | H |
| ATOM | 6263 | O | HOH H 299 | 70.560 | 48.918 | 1.476 | 1.00 | 49.72 | H |
| ATOM | 6264 | O | HOH H 300 | 84.037 | 38.916 | 5.971 | 1.00 | 39.33 | H |
| ATOM | 6265 | O | HOH H 301 | 86.468 | 41.381 | 11.971 | 1.00 | 45.69 | H |
| ATOM | 6266 | O | HOH H 302 | 24.400 | 11.569 | 23.610 | 1.00 | 36.73 | H |
| ATOM | 6267 | O | HOH H 303 | 73.087 | 79.808 | 7.028 | 1.00 | 46.20 | H |
| ATOM | 6268 | O | HOH H 304 | 72.681 | 43.116 | 14.941 | 1.00 | 51.84 | H |
| ATOM | 6269 | O | HOH H 305 | 84.844 | 42.198 | 15.611 | 1.00 | 26.23 | H |
| ATOM | 6270 | O | HOH H 306 | 54.135 | 19.007 | 24.978 | 1.00 | 27.41 | H |
| ATOM | 6271 | O | HOH H 307 | 67.044 | 10.459 | 18.465 | 1.00 | 44.92 | H |
| ATOM | 6272 | O | HOH H 308 | 82.262 | 49.436 | 14.864 | 1.00 | 39.04 | H |
| ATOM | 6273 | O | HOH H 309 | 114.093 | 50.994 | 16.895 | 1.00 | 43.32 | H |
| ATOM | 6274 | O | HOH H 310 | 64.428 | 3.092 | 30.590 | 1.00 | 43.29 | H |
| ATOM | 6275 | O | HOH H 311 | 81.152 | 70.187 | 18.656 | 1.00 | 34.21 | H |
| ATOM | 6276 | O | HOH H 312 | 74.596 | 81.584 | -2.515 | 1.00 | 55.00 | H |
| ATOM | 6277 | O | HOH H 313 | 61.161 | 25.774 | 22.464 | 1.00 | 32.98 | H |
| ATOM | 6278 | O | HOH H 314 | 53.149 | -7.019 | 4.754 | 1.00 | 26.01 | H |
| ATOM | 6279 | O | HOH H 315 | 44.571 | 8.317 | 33.567 | 1.00 | 40.32 | H |
| ATOM | 6280 | O | HOH H 316 | 82.293 | 49.769 | 10.587 | 1.00 | 35.22 | H |
| ATOM | 6281 | O | HOH H 317 | 48.467 | 8.859 | 24.614 | 1.00 | 42.38 | H |
| ATOM | 6282 | O | HOH H 318 | 56.588 | -8.027 | 4.728 | 1.00 | 44.65 | H |
| ATOM | 6283 | O | HOH H 319 | 31.280 | -23.239 | 26.551 | 1.00 | 42.45 | H |
| ATOM | 6284 | O | HOH H 320 | 82.483 | 40.137 | 7.719 | 1.00 | 39.22 | H |
| ATOM | 6285 | O | HOH H 321 | 82.063 | 19.937 | 23.440 | 1.00 | 35.69 | H |

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ATOM   6286  O   HOH H 322   106.025  63.366  22.616  1.00 31.93      H
ATOM   6287  O   HOH H 323    46.181   9.890   8.669  1.00 38.11      H
ATOM   6288  O   HOH H 324    71.708  75.568   6.998  1.00 41.82      H
ATOM   6289  O   HOH H 325   108.280  34.405   3.851  1.00 30.72      H
ATOM   6290  O   HOH H 326    32.275  40.921  14.635  1.00 40.72      H
ATOM   6291  O   HOH H 327    37.556  15.785   5.690  1.00 42.29      H
ATOM   6292  O   HOH H 328    85.569  33.598  37.182  1.00 31.78      H
ATOM   6293  O   HOH H 329    33.070 -11.287  23.137  1.00 48.90      H
ATOM   6294  O   HOH H 330    87.593  16.513  19.683  1.00 45.53      H
ATOM   6295  O   HOH H 331   116.176  53.631  17.853  1.00 39.81      H
ATOM   6296  O   HOH H 332    26.940 -11.377  14.930  1.00 39.40      H
ATOM   6297  O   HOH H 333    60.033  28.679  22.456  1.00 32.84      H
ATOM   6298  O   HOH H 334    52.472  15.182   2.562  1.00 48.72      H
ATOM   6299  O   HOH H 335    84.377  54.588   4.646  1.00 40.99      H
ATOM   6300  O   HOH H 336   115.759  67.454  19.970  1.00 46.15      H
ATOM   6301  O   HOH H 337    88.969  52.684  25.112  1.00 42.31      H
ATOM   6302  O   HOH H 338    36.351  12.852   9.875  1.00 37.11      H
ATOM   6303  O   HOH H 339    97.702  31.578   2.653  1.00 49.82      H
ATOM   6304  O   HOH H 340    53.964  -6.543  26.981  1.00 35.52      H
ATOM   6305  O   HOH H 341    24.475 -17.438  17.094  1.00 38.04      H
ATOM   6306  O   HOH H 342    58.530   0.915  19.036  1.00 43.08      H
ATOM   6307  O   HOH H 343    77.156  37.203  39.025  1.00 48.54      H
ATOM   6308  O   HOH H 344    49.978  -1.361   0.435  1.00 39.48      H
ATOM   6309  O   HOH H 345    53.900  37.104  13.703  1.00 47.74      H
ATOM   6310  O   HOH H 346    77.886  49.625  13.575  1.00 57.13      H
ATOM   6311  O   HOH H 347    57.053   8.721   0.570  1.00 50.38      H
ATOM   6312  O   HOH H 348    96.803  63.745  10.854  1.00 41.14      H
ATOM   6313  O   HOH H 349    89.009  70.808  11.906  1.00 45.67      H
ATOM   6314  O   HOH H 350    66.363  22.353   8.221  1.00 42.47      H
ATOM   6315  O   HOH H 351    52.578  25.044   8.541  1.00 41.16      H
ATOM   6316  O   HOH H 352    81.789  73.640  -3.536  1.00 50.48      H
ATOM   6317  O   HOH H 353    67.632 -11.181  13.891  1.00 48.24      H
ATOM   6318  O   HOH H 354    41.357  -5.652  22.367  1.00 14.47      H
ATOM   6319  C1  EDO G 501    37.685  -5.096  30.876  1.00 23.96      G
ATOM   6320  O1  EDO G 501    38.224  -4.213  31.883  1.00 23.38      G
ATOM   6321  C2  EDO G 501    38.742  -6.046  30.406  1.00 25.29      G
ATOM   6322  O2  EDO G 501    39.062  -6.931  31.464  1.00 26.30      G
ATOM   6323  C1  EDO G 502    89.146  26.377  27.000  1.00 41.69      G
ATOM   6324  O1  EDO G 502    88.631  26.508  28.343  1.00 51.10      G
ATOM   6325  C2  EDO G 502    88.436  25.261  26.303  1.00 43.14      G
ATOM   6326  O2  EDO G 502    88.726  24.052  26.967  1.00 41.73      G
ATOM   6327  C1  EDO G 503    85.093  31.920  30.633  1.00 21.00      G
ATOM   6328  O1  EDO G 503    85.283  30.597  31.203  1.00 18.65      G
ATOM   6329  C2  EDO G 503    83.846  32.561  31.186  1.00 19.69      G
ATOM   6330  O2  EDO G 503    84.148  33.101  32.454  1.00 20.94      G
ATOM   6331  C1  EDO G 504    34.956   3.907  25.885  1.00 38.01      G
ATOM   6332  O1  EDO G 504    33.976   2.838  25.869  1.00 36.69      G
ATOM   6333  C2  EDO G 504    36.360   3.344  25.982  1.00 39.84      G
ATOM   6334  O2  EDO G 504    36.573   2.396  24.935  1.00 33.51      G
END
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## Example 4

[91]     Binding of altered gluten peptides (peptide analogs) to MHC molecules is assayedwith purified HLA molecules. Binding of labeled peptide to purified HLA DQ2 molecules can be measured as described by Johansen et al. (1996) Int Immmunol (8), 177-82. Briefly, purified DQ2 molecules (50 - 1000 nM) are incubated with the 125-I radiolabeled indicator peptide (MB 65kDa 243-255Y, sequence KPLLIIAEDVEGEY; 20 000 cpm, 1-5 nM) at pH 4.9. After incubation for 24 hours, the peptide bound to DQ2 and the non-bound peptide are separated on Sephadex G25 superfine spun columns. The radioactivity in the bound and non-bound fractions was counted in a gamma-counter, and the fraction of peptide bound to DQ2 (cpm in the bound fraction/total cpm recovered) is calculated. The binding capacities of the peptide binding inhibitors are assayed by testing their ability to inhibit the binding of the labeled indicator peptide. The concentration required to give 50%

inhibition ($IC_{50}$) is calculated. Since the level of $IC_{50}$ may vary between separate titration experiments, the $IC_{50}$ values are compared to the $IC_{50}$ of a reference peptide by determining the relative binding capacity (RBC), which is the ratio: $IC_{50}$ of reference peptide / $IC_{50}$ of test compound. HLA-DQ2 molecules can be isolated by antibody affinity chromatography from lysates of HLA-DQ2 homozygous Epstein Barr virus transformed B-lymphoblastoid cell lines (detergent solubilized) or from water soluble, recombinant molecules produced similarly as described in Example 3 above. The recombinant molecules can be made with or without covalently linked peptide and with a biotin recognition sequence at the C-terminal end of the β-subunit that facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling alternative ways for measurement of $IC_{50i}$. A peptide analog with an $IC_{50}$ value of less than 100 μM is suitable for further screenings.

[92]     Alternatively, binding of altered gluten peptides to HLA-DQ2 can also be assayed using the soluble DQ2 heterodimer produced as described in Example 3 above. The presence of the biotin recognition sequence at the C-terminal end of the β-subunit facilitates adsorption of HLA-DQ2 to several streptavidin coated supports, thereby enabling measurement of $IC_{50}$ or $K_i$.

[93]     Candidate peptide analogs are further tested for their ability to inhibit proliferation of T cells specific for gluten peptides.   This is done by using HLA-DQ2 restricted T cell clones (TCC) and glutaraldehyde fixed antigen presenting cells (e.g. Epstein Barr virus transformed B-lymphoid transformed cells) expressing HLA-DQ2. The antigen presenting cells are pelleted and resuspended in RPMI containing 0.05% glutaraldehyde for 90 sec, whereafter glycin to a final concentration of 0.2 M is added for 60 sec. The cells are then washed, counted, and resuspended in PBS or PBS buffered with citrate phosphate to a final pH of 4.9. The fixed APC are incubated overnight with various concentrations of peptides. The inhibitory peptides are usually added 30 min prior to the stimulatory peptide. The antigen presenting cells are then washed twice and resuspended in culture medium of RPMI-1640 supplemented with 15% v/v heat inactivated pooled human serum and the T cells are added. The experiments are performed in triplicates of 3-5 X $10^4$ TCC with 5 X $10^4$ fixed APC and various titrations of inhibitory and stimulatory peptides. Following an incubation period of 48 hours, each culture is pulsed with [$^3$H]-thymidine for an additional 12-18 hours. Cultures are then harvested on fiberglass filters and counted as above. Mean CPM and standard error of the mean are calculated from data determined in triplicate cultures. Peptide analogs that inhibit proliferation to approximately 25% at a concentration of 50 μM or greater are suitable for further screening.

[94]     All publications and patent applications cited in this specification are herein incorporated by reference as if each individual publication or patent application were specifically and individually indicated to be incorporated by reference.

[95]     Although the foregoing invention has been described in some detail by way of illustration and example for purposes of clarity of understanding, it will be readily apparent to those of ordinary skill in the art in light of the teachings of this invention that certain changes and modifications may be made thereto without departing from the spirit or scope of the appended claims.

WHAT IS CLAIMED IS:

1.    An HLA-binding peptide inhibitor; wherein said inhibitor is an analog of an immunogenic gluten oligopeptide of at least about 8 residues in length, wherein the immunogenic gluten oligopeptide is altered by the replacement of one or more amino acids; and wherein said analog binds tightly to HLA molecules; is proteolytically stable; and does not activate disease-specific T cells.

2.    The HLA-binding peptide inhibitor of Claim 1, wherein said analog comprises one or more naturally occurring amino acids, non-naturally occurring amino acids, modified amino acids, or amino acid mimetics.

3.    The HLA-binding peptide inhibitor of Claim 2, wherein said analog is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

4.    The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises at least one PXP motif.

5.    The HLA-binding peptide inhibitor of Claim 1, wherein said immunogenic gluten oligopeptides comprises a sequence selected from the group consisting of: PQPELPY; PFPQPELPYP, PQPELPYPQPQLP, PQQSFPEQQPP, VQGQGIIQPEQPAQ, FPEQPQQPYPQQP, FPQQPEQPYPQQP, FSQPEQEFPQPQ; PFPQPQLPY, PQPQLPYPQ, PFPQPELPY; PYPQPELPY and PYPQPQLPY.

[96]    6.    The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PXPQPELPY, where X is Tyr, Trp, Arg, Lys, p-iodo-Phe, 3-iodo-Tyr, p-amino-Phe, 3-amino-Tyr, hydroxylysine, ornithine, Asp or Glu.

7.    The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

8.    The HLA-binding peptide inhibitor of Claim 6, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.

9.    The HLA-binding peptide inhibitor of Claim 1, wherein said inhibitor comprises the sequence PFPQX$_1$ELX$_2$Y, where X$_1$ and X$_2$ are independently selected from 4-hydroxy-Pro, 4-amino-Pro, or 3-hydroxy-Pro, and proline, with the proviso that at least one of X$_1$ and X$_2$ is a residue other than proline

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10.     The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further derivatized to reduce the affinity of the analog for disease-specific T cell receptors.

11.     The HLA-binding peptide inhibitor of Claim 9, wherein said inhibitor is further modified to increase binding potency to an MHC molecule.

12.     A method of treating Celiac Sprue and/or dermatitis herpetiformis, the method comprising:
        administering to a patient an effective dose of an HLA-binding peptide inhibitor;
        wherein said HLA-binding peptide inhibitor attenuates gluten toxicity in said patient.

13.     The method of Claim 12, wherein said HLA-binding peptide inhibitor is administered with a glutenase.

14.     The method according to Claim 12, wherein said HLA-binding peptide inhibitor is administered orally.

15.     The method according to Claim 12, wherein said HLA-binding peptide inhibitor is contained in a formulation that comprises an enteric coating.

16.     A formulation for use in treatment of Celiac Sprue and/or dermatitis herpetiformis, comprising:
        an effective dose of an HLA-binding peptide inhibitor and a pharmaceutically acceptable excipient.

17.     The formulation according to Claim 16, further comprising an enteric coating.

18.     Use of an HLA-binding peptide inhibitor in the treatment of HLA-DQ2 positive individuals who are either pre-disposed to type I diabetes or have developed symptoms of type I diabetes.

19.     A computer for producing a three-dimensional representation of a molecule wherein said molecule comprises an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, wherein said computer comprises:
        a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic

gluten oligopeptide;

a working memory for storing instructions for processing said machine-readable data;

a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

a display coupled to said central-processing unit for displaying said three-dimensional representation.


20.      A computer-assisted method for identifying potential modulators of Celiac Sprue and/or dermatitis herpetiformis, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:

(a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in an HLA-DQ2 molecule bound to an immunogenic gluten oligopeptide, thereby generating a criteria data set;

(b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;

(c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;

(d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.